Computing the Laplacian of $f(x, y, z) = x^2 + y^2 + z^2$

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Abstract

This document demonstrates the computation of the Laplacian of the function $f(x, y, z) = x^2 + y^2 + z^2$ using both the continuous and discrete forms in three dimensions, with an extension to two dimensions. The continuous form involves summing second partial derivatives, while the discrete form uses the difference between the function's value and its average over a small sphere or circle. Computations are performed at multiple points, and results are interpreted geometrically and physically. Additional examples and a comparison of the 2D and 3D cases enhance understanding of the Laplacian's significance.

1 Introduction

The Laplacian operator ∇^2 quantifies the local curvature of a scalar function, playing a critical role in physics and mathematics, such as in diffusion, electrostatics, and harmonic analysis. For the function $f(x, y, z) = x^2 + y^2 + z^2$, we compute the Laplacian using:

- **Continuous form**: Sum of second partial derivatives.
- **Discrete form**: Scaled difference between the function's value and its average over a small neighborhood.

This document verifies that both forms yield consistent results, provides intuitive interpretations, and extends the analysis to additional points and dimensions.

2 Function and Laplacian Definitions

Consider the function:

$$f(x, y, z) = x^2 + y^2 + z^2.$$

This is a radially symmetric function representing the squared distance from the origin, resembling a paraboloid opening upward.

2.1 Continuous Laplacian

In 3D Cartesian coordinates:

$$\nabla^2 f = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} + \frac{\partial^2 f}{\partial z^2}.$$

In 2D (for comparison):

$$\nabla^2 f = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2}.$$

2.2 Discrete Laplacian

In 3D, over a sphere of radius dx:

$$\nabla^2 f(x_0) = \lim_{dx\to 0} 6\frac{\langle f\rangle_{\text{around}} - f(x_0)}{dx^2},$$

where $\langle f\rangle_{\text{around}}$ is the average of f over the sphere's surface. In 2D, over a circle:

$$\nabla^2 f(x_0) = \lim_{dx\to 0} 4\frac{\langle f\rangle_{\text{around}} - f(x_0)}{dx^2}.$$

3 Computation in 3D

3.1 Continuous Form at $x_0 = (0,0,0)$

Compute the second partial derivatives:

$$\begin{aligned}
\frac{\partial f}{\partial x} &= 2x, & \frac{\partial^2 f}{\partial x^2} &= 2,\\
\frac{\partial f}{\partial y} &= 2y, & \frac{\partial^2 f}{\partial y^2} &= 2,\\
\frac{\partial f}{\partial z} &= 2z, & \frac{\partial^2 f}{\partial z^2} &= 2.
\end{aligned}$$

Sum:

$$\nabla^2 f = 2+2+2 = 6.$$

The Laplacian is constant, reflecting the uniform curvature of the paraboloid.

3.2 Discrete Form at $x_0 = (0,0,0)$

Evaluate $f(x_0) = f(0,0,0) = 0$. Compute the average over a sphere of radius dx:

$$\langle f\rangle_{\text{around}} = \frac{1}{4\pi dx^2}\int_S (x^2+y^2+z^2)\,dS.$$

On the sphere, $x^2+y^2+z^2 = dx^2$. Thus:

$$\langle f\rangle_{\text{around}} = \frac{1}{4\pi dx^2}\int_S dx^2\,dS = \frac{dx^2\cdot 4\pi dx^2}{4\pi dx^2} = dx^2.$$

Apply the discrete formula:

$$\nabla^2 f \approx 6\frac{\langle f\rangle_{\text{around}} - f(x_0)}{dx^2} = 6\frac{dx^2-0}{dx^2} = 6.$$

In the limit $dx \to 0$:

$$\nabla^2 f = 6.$$

This matches the continuous result.

3.3 Continuous Form at $x_0 = (1, 1, 1)$

The second derivatives are the same, so:

$$\nabla^2 f = 6.$$

The Laplacian is constant everywhere, as f has uniform curvature.

3.4 Discrete Form at $x_0 = (1, 1, 1)$

Evaluate $f(1, 1, 1) = 1^2 + 1^2 + 1^2 = 3$. For a sphere centered at $(1, 1, 1)$, parameterize points as:

$$(x, y, z) = (1 + dx \sin\theta \cos\phi, 1 + dx \sin\theta \sin\phi, 1 + dx \cos\theta).$$

Compute:

$$f = (1 + dx \sin\theta \cos\phi)^2 + (1 + dx \sin\theta \sin\phi)^2 + (1 + dx \cos\theta)^2.$$

Expand:

$$(1 + dx \sin\theta \cos\phi)^2 \approx 1 + 2dx \sin\theta \cos\phi + dx^2 \sin^2\theta \cos^2\phi,$$

and similarly for other terms. Sum:

$$f \approx 3 + 2dx(\sin\theta \cos\phi + \sin\theta \sin\phi + \cos\theta) + dx^2(\sin^2\theta \cos^2\phi + \sin^2\theta \sin^2\phi + \cos^2\theta).$$

Integrate over the sphere:

$$\langle f \rangle_{\text{around}} = \frac{1}{4\pi} \int_0^{\pi} \int_0^{2\pi} f \sin\theta \, d\theta \, d\phi.$$

The linear terms vanish (symmetry of $\hat{n}$):

$$\int_0^{\pi} \int_0^{2\pi} \sin\theta \cos\phi \sin\theta \, d\theta \, d\phi = 0, \quad \text{etc.}$$

The quadratic term:

$$\sin^2\theta \cos^2\phi + \sin^2\theta \sin^2\phi + \cos^2\theta = \sin^2\theta + \cos^2\theta = 1.$$

Thus:

$$\langle f \rangle_{\text{around}} \approx 3 + dx^2 \cdot \frac{1}{4\pi} \int_0^{\pi} \int_0^{2\pi} 1 \cdot \sin\theta \, d\theta \, d\phi = 3 + dx^2.$$

Apply the discrete formula:

$$\nabla^2 f \approx 6 \frac{(3 + dx^2) - 3}{dx^2} = 6 \frac{dx^2}{dx^2} = 6.$$

In the limit:

$$\nabla^2 f = 6.$$

4 Computation in 2D

Consider $f(x, y) = x^2 + y^2$ in 2D.

4.1 Continuous Form at $(0,0)$

$$\frac{\partial f}{\partial x} = 2x, \quad \frac{\partial^2 f}{\partial x^2} = 2, \quad \frac{\partial f}{\partial y} = 2y, \quad \frac{\partial^2 f}{\partial y^2} = 2.$$

$$\nabla^2 f = 2 + 2 = 4.$$

4.2 Discrete Form at $(0,0)$

Evaluate $f(0,0) = 0$. Over a circle of radius dx:

$$\langle f \rangle_{\text{around}} = \frac{1}{2\pi dx} \int_C (x^2 + y^2)\, dl.$$

On the circle, $x^2 + y^2 = dx^2$:

$$\langle f \rangle_{\text{around}} = \frac{1}{2\pi dx} \int_0^{2\pi} dx^2 \cdot dx\, d\theta = dx^2.$$

$$\nabla^2 f \approx 4\frac{dx^2 - 0}{dx^2} = 4.$$

In the limit:

$$\nabla^2 f = 4.$$

5 Intuitive Explanation

The Laplacian measures how f at a point compares to its average over a small neighborhood:

- **Positive Laplacian ($\nabla^2 f = 6$ in 3D, 4 in 2D)**: At $(0,0,0)$, $f = 0$, but the average over the sphere is $dx^2 > 0$. This indicates f is in a "valley" (convex, like a paraboloid).
- **Geometric Insight**: The function $f = x^2 + y^2 + z^2$ is a paraboloid, curving upward uniformly. The constant Laplacian reflects this consistent curvature.
- **Physical Meaning**: In diffusion, a positive Laplacian suggests the function (e.g., concentration) is lower at the point than its surroundings, driving inward flow. In electrostatics, it implies a negative charge density via Poisson's equation.

The factors 6 (3D) and 4 (2D) arise from the geometry of the sphere and circle, respectively, scaling the curvature measurement appropriately for the dimension.

6 Additional Example: Non-Zero Laplacian at a Different Point

Consider $f(x, y, z) = x^2 - y^2 + z^2$ at $(0,0,0)$.

6.1 Continuous Form

$$\frac{\partial^2 f}{\partial x^2} = 2, \quad \frac{\partial^2 f}{\partial y^2} = -2, \quad \frac{\partial^2 f}{\partial z^2} = 2.$$

$$\nabla^2 f = 2 - 2 + 2 = 2.$$

6.2 Discrete Form

Evaluate $f(0,0,0) = 0$. On the sphere:

$$f = (dx \sin\theta \cos\phi)^2 - (dx \sin\theta \sin\phi)^2 + (dx \cos\theta)^2.$$

$$= dx^2(\sin^2\theta \cos^2\phi - \sin^2\theta \sin^2\phi + \cos^2\theta).$$

Compute the average:

$$\langle f \rangle_{\text{around}} = \frac{1}{4\pi} \int_0^{\pi} \int_0^{2\pi} dx^2(\sin^2\theta \cos^2\phi - \sin^2\theta \sin^2\phi + \cos^2\theta) \sin\theta \, d\theta \, d\phi.$$

Split integrals:

$$\int_0^{2\pi} (\cos^2\phi - \sin^2\phi) \, d\phi = \int_0^{2\pi} \cos 2\phi \, d\phi = 0,$$

$$\int_0^{\pi} \cos^2\theta \sin\theta \, d\theta = \int_0^{\pi} \frac{1 - \sin^2\theta}{2} \sin\theta \, d\theta = \frac{1}{3}.$$

This requires careful integration, but the Hessian trace gives:

$$\langle f \rangle_{\text{around}} \approx \frac{dx^2}{3} \cdot 2 = \frac{2dx^2}{3}.$$

$$\nabla^2 f \approx 6 \frac{\frac{2dx^2}{3} - 0}{dx^2} = 2.$$

In the limit:

$$\nabla^2 f = 2.$$

7 Applications

- **Diffusion**: The positive Laplacian of $f = x^2 + y^2 + z^2$ indicates a region where a quantity (e.g., heat) flows inward.
- **Electrostatics**: In Poisson's equation, $\nabla^2 \phi = 6$ suggests a negative charge density.
- **Numerical Methods**: The discrete form is the basis for finite-difference approximations in computational physics.

8 Summary

For $f(x, y, z) = x^2 + y^2 + z^2$, both the continuous ($\nabla^2 f = 6$) and discrete forms yield consistent results in 3D, with $\nabla^2 f = 4$ in 2D. The positive Laplacian reflects the function's convex, paraboloid shape. Computations at different points and for a modified function confirm the methods' robustness. The Laplacian's geometric and physical interpretations highlight its role in describing curvature and dynamics.

Computing the Laplacian of Functions with Two or Three Variables

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Abstract

This document presents two methods for computing the Laplacian $\nabla^2 f$ of a scalar function f with two or three variables: (1) direct computation in Cartesian coordinates and (2) transformation to polar or spherical coordinates. Each method is explained with mathematical formulations, practical considerations, and examples. These approaches are fundamental in fields such as physics, engineering, and applied mathematics.

1 Introduction

The Laplacian operator ∇^2 is a second-order differential operator that measures the divergence of the gradient of a scalar function f. For a function f with two or three variables, the Laplacian quantifies how the function changes spatially, making it essential in applications like heat conduction, electrostatics, and fluid dynamics. This document outlines two distinct methods to compute $\nabla^2 f$, highlighting their advantages and use cases.

2 Method 1: Direct Computation in Cartesian Coordinates

The simplest and most straightforward method to compute the Laplacian is to apply the operator directly in Cartesian coordinates.

2.1 Formulation

For a scalar function f:

- In **two dimensions** (x, y), the Laplacian is:

$$\nabla^2 f = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2}$$

- In **three dimensions** (x, y, z), the Laplacian is:

$$\nabla^2 f = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} + \frac{\partial^2 f}{\partial z^2}$$

2.2 Procedure

1. Compute the second partial derivative of f with respect to each variable.
2. Sum the second partial derivatives to obtain $\nabla^2 f$.

2.3 Advantages

- Intuitive and aligns with the standard definition of the Laplacian.
- Requires no coordinate transformation, making it computationally simple for functions defined in Cartesian coordinates.
- Applicable to any differentiable function, regardless of symmetry.

2.4 Example: Two Dimensions

Consider $f(x, y) = x^2 + y^2$.

1. Compute second partial derivatives:

$$\frac{\partial f}{\partial x} = 2x, \quad \frac{\partial^2 f}{\partial x^2} = 2$$

$$\frac{\partial f}{\partial y} = 2y, \quad \frac{\partial^2 f}{\partial y^2} = 2$$

2. Sum the second derivatives:

$$\nabla^2 f = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} = 2 + 2 = 4$$

Result: $\nabla^2 f = 4$.

2.5 Example: Three Dimensions

Consider $f(x, y, z) = x^2 + y^2 + z^2$.

1. Compute second partial derivatives:

$$\frac{\partial f}{\partial x} = 2x, \quad \frac{\partial^2 f}{\partial x^2} = 2$$

$$\frac{\partial f}{\partial y} = 2y, \quad \frac{\partial^2 f}{\partial y^2} = 2$$

$$\frac{\partial f}{\partial z} = 2z, \quad \frac{\partial^2 f}{\partial z^2} = 2$$

2. Sum the second derivatives:

$$\nabla^2 f = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} + \frac{\partial^2 f}{\partial z^2} = 2 + 2 + 2 = 6$$

Result: $\nabla^2 f = 6$.

2.6 Limitations

- May become cumbersome for functions with complex expressions.
- Inefficient for problems with radial or angular symmetry, where polar or spherical coordinates simplify the computation.

3 Method 2: Coordinate Transformation (Polar or Spherical Coordinates)

For functions exhibiting radial or angular symmetry, transforming the function into polar (2D) or spherical (3D) coordinates can simplify the computation of the Laplacian.

3.1 Formulation

The Laplacian operator changes depending on the coordinate system.

3.1.1 Polar Coordinates (2D)

In polar coordinates (r, θ), where $x = r\cos\theta$, $y = r\sin\theta$, the Laplacian of a function $f(r, \theta)$ is:

$$\nabla^2 f = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial f}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 f}{\partial \theta^2} \tag{1}$$

This can be expanded as:

$$\nabla^2 f = \frac{\partial^2 f}{\partial r^2} + \frac{1}{r}\frac{\partial f}{\partial r} + \frac{1}{r^2}\frac{\partial^2 f}{\partial \theta^2}$$

3.1.2 Spherical Coordinates (3D)

In spherical coordinates (r, θ, ϕ), where $x = r\sin\theta\cos\phi$, $y = r\sin\theta\sin\phi$, $z = r\cos\theta$, the Laplacian of a function $f(r, \theta, \phi)$ is:

$$\nabla^2 f = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial f}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta\frac{\partial f}{\partial \theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2 f}{\partial \phi^2} \tag{2}$$

For a radially symmetric function $f(r)$, this simplifies to:

$$\nabla^2 f(r) = \frac{2}{r}\frac{\partial f}{\partial r} + \frac{\partial^2 f}{\partial r^2}$$

3.2 Procedure

1. Express the function f in polar or spherical coordinates by substituting the appropriate coordinate transformations.
2. Compute the partial derivatives as required by the Laplacian formula in the chosen coordinate system.
3. Simplify the expression, leveraging symmetry if applicable.

3.3 Advantages

- Simplifies calculations for functions with radial or angular symmetry (e.g., $f(r)$ in 3D or $f(r,\theta)$ in 2D).
- Reduces the number of terms in problems with spherical or cylindrical symmetry.
- Commonly used in physics for problems like the Coulomb potential or wavefunctions.

3.4 Example: Two Dimensions (Polar Coordinates)

Consider $f(x,y) = x^2 + y^2$. In polar coordinates, $x = r\cos\theta$, $y = r\sin\theta$, so:

$$f(r,\theta) = (r\cos\theta)^2 + (r\sin\theta)^2 = r^2(\cos^2\theta + \sin^2\theta) = r^2$$

Compute the Laplacian:

1. Partial derivatives with respect to r:

$$\frac{\partial f}{\partial r} = \frac{\partial}{\partial r}(r^2) = 2r, \quad \frac{\partial^2 f}{\partial r^2} = 2$$

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial f}{\partial r}\right) = \frac{1}{r}\frac{\partial}{\partial r}(r \cdot 2r) = \frac{1}{r}\frac{\partial}{\partial r}(2r^2) = \frac{1}{r} \cdot 4r = 4$$

2. Partial derivatives with respect to θ:

$$\frac{\partial f}{\partial \theta} = 0, \quad \frac{\partial^2 f}{\partial \theta^2} = 0$$

3. Combine:

$$\nabla^2 f = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial f}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 f}{\partial \theta^2} = 4 + 0 = 4$$

Result: $\nabla^2 f = 4$, matching the Cartesian result.

3.5 Example: Three Dimensions (Spherical Coordinates)

Consider $f(x,y,z) = x^2 + y^2 + z^2$. In spherical coordinates, $r = \sqrt{x^2 + y^2 + z^2}$, so:

$$f(r) = r^2$$

Since f depends only on r, use the simplified Laplacian:

1. Compute derivatives:

$$\frac{\partial f}{\partial r} = 2r, \quad \frac{\partial^2 f}{\partial r^2} = 2$$

2. Apply the formula:

$$\nabla^2 f = \frac{2}{r}\frac{\partial f}{\partial r} + \frac{\partial^2 f}{\partial r^2} = \frac{2}{r}(2r) + 2 = 4 + 2 = 6$$

Result: $\nabla^2 f = 6$, matching the Cartesian result.

3.6 Limitations

- Requires transforming the function into the new coordinate system, which can be complex for non-symmetric functions.
- Singularities (e.g., at $r = 0$ or $\theta = 0, \pi$) may complicate calculations.
- More involved for functions without clear symmetry.

4 Comparison of Methods

Table 1: Comparison of Laplacian Computation Methods

Aspect	**Cartesian**	**Polar/Spherical**
Simplicity	High	Moderate
Best for	General functions	Symmetric functions
Coordinate Transformation	None	Required
Handling Singularities	None	Possible (e.g., $r = 0$)
Computational Effort	Low	Higher for non-symmetric cases

5 Conclusion

The Laplacian of a function with two or three variables can be computed effectively using either direct computation in Cartesian coordinates or transformation to polar/spherical coordinates. The Cartesian method is straightforward and universally applicable, while the coordinate transformation method excels in problems with radial or angular symmetry. The choice of method depends on the function's form and the problem's context, with both approaches yielding consistent results when applied correctly.

Derivation and Interpretation of the Laplacian Operator

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Abstract

This document derives the discrete form of the Laplacian operator in two and three dimensions, showing its equivalence to the standard continuous form in Cartesian coordinates. The discrete form expresses the Laplacian as a scaled difference between a function's value at a point and its average over an infinitesimal sphere or circle. Detailed derivations, intuitive explanations, and examples in 2D and 3D are provided, along with applications in physics. The document emphasizes the geometric and physical significance of the Laplacian as a measure of local curvature or deviation from harmonicity.

1 Introduction

The Laplacian operator ∇^2 is a fundamental tool in mathematics and physics, quantifying the divergence of the gradient of a scalar function f. It appears in equations governing diffusion, electrostatics, and wave propagation. The Laplacian has two equivalent representations:

- **Continuous form**: The sum of second partial derivatives in Cartesian coordinates.
- **Discrete form**: A limit involving the difference between the function's value at a point and its average over a small neighborhood.

This document derives the discrete form in 2D and 3D, provides intuitive interpretations, and illustrates its application through examples.

2 Laplacian Expressions

2.1 Continuous Form

In Cartesian coordinates:

- In two dimensions (x, y):
$$\nabla^2 f = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2}$$
- In three dimensions (x, y, z):
$$\nabla^2 f = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} + \frac{\partial^2 f}{\partial z^2}$$

2.2 Discrete Form

The discrete form expresses the Laplacian as a limit involving the average of f over a small neighborhood:

- In two dimensions (circle of radius dx):

$$\nabla^2 f(x) = \lim_{dx \to 0} 4 \frac{\langle f \rangle_{\text{around}} - f(x_0)}{dx^2}$$

- In three dimensions (sphere of radius dx):

$$\nabla^2 f(x) = \lim_{dx \to 0} 6 \frac{\langle f \rangle_{\text{around}} - f(x_0)}{dx^2}$$

Here, $\langle f \rangle_{\text{around}}$ is the average value of f over a circle (2D) or sphere (3D) of radius dx centered at x_0.

3 Derivation of the Discrete Form

3.1 Three Dimensions

Consider a scalar function $f(x, y, z)$ at point x_0. The average value of f over the surface of a sphere of radius dx centered at x_0 is:

$$\langle f \rangle_{\text{around}} = \frac{1}{4\pi dx^2} \int_S f(x_0 + dx \cdot \hat{n})\, dS, \tag{1}$$

where S is the sphere's surface, $\hat{n}$ is the unit normal vector, and $4\pi dx^2$ is the surface area of the sphere.

Expand $f(x_0 + dx \cdot \hat{n})$ using a Taylor series around x_0:

$$f(x_0 + dx \cdot \hat{n}) \approx f(x_0) + dx \cdot \nabla f(x_0) \cdot \hat{n} + \frac{dx^2}{2} \hat{n}^T H \hat{n} + O(dx^3), \tag{2}$$

where H is the Hessian matrix of f, with elements $H_{ij} = \frac{\partial^2 f}{\partial x_i \partial x_j}$.

Integrate each term over the sphere:

1. **Constant term**: $f(x_0)$ is constant, so:

$$\frac{1}{4\pi dx^2} \int_S f(x_0)\, dS = f(x_0).$$

2. **Linear term**: The gradient term $dx \cdot \nabla f(x_0) \cdot \hat{n}$ averages to zero because $\hat{n}$ is symmetric over the sphere:

$$\int_S \hat{n}\, dS = 0.$$

3. **Quadratic term**: The term $\hat{n}^T H \hat{n} = \sum_{i,j} H_{ij} n_i n_j$. The average over the sphere is:

$$\langle n_i n_j \rangle = \frac{1}{4\pi} \int n_i n_j \, d\Omega = \frac{1}{3} \delta_{ij},$$

where $d\Omega$ is the solid angle element. Thus:

$$\langle \hat{n}^T H \hat{n} \rangle = \sum_{i,j} H_{ij} \langle n_i n_j \rangle = \sum_{i,j} H_{ij} \cdot \frac{1}{3}\delta_{ij} = \frac{1}{3} \sum_i H_{ii} = \frac{1}{3}\mathrm{Tr}(H).$$

Since $\mathrm{Tr}(H) = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} + \frac{\partial^2 f}{\partial z^2} = \nabla^2 f$, the quadratic term contributes:

$$\frac{dx^2}{2} \cdot \frac{1}{3}\nabla^2 f = \frac{dx^2}{6}\nabla^2 f.$$

Combining:

$$\langle f \rangle_{\text{around}} \approx f(x_0) + \frac{dx^2}{6}\nabla^2 f(x_0).$$

Rearrange:

$$\nabla^2 f(x_0) \approx \frac{6}{dx^2}\left(\langle f \rangle_{\text{around}} - f(x_0)\right).$$

Taking the limit $dx \to 0$:

$$\nabla^2 f(x_0) = \lim_{dx \to 0} 6 \frac{\langle f \rangle_{\text{around}} - f(x_0)}{dx^2}. \tag{3}$$

3.2 Two Dimensions

In 2D, consider a circle of radius dx centered at x_0. The average is:

$$\langle f \rangle_{\text{around}} = \frac{1}{2\pi dx} \int_C f(x_0 + dx \cdot \hat{n})\, dl,$$

where C is the circle's circumference, and $2\pi dx$ is its length. The Taylor expansion is similar:

$$f(x_0 + dx \cdot \hat{n}) \approx f(x_0) + dx \cdot \nabla f(x_0) \cdot \hat{n} + \frac{dx^2}{2}\hat{n}^T H \hat{n} + O(dx^3).$$

Integrate:

1. **Constant term**: $f(x_0)$.
2. **Linear term**: Averages to zero due to symmetry.
3. **Quadratic term**: In 2D, $\langle n_i n_j \rangle = \frac{1}{2}\delta_{ij}$, so:

   $$\langle \hat{n}^T H \hat{n} \rangle = \frac{1}{2}\mathrm{Tr}(H) = \frac{1}{2}\nabla^2 f.$$

   The quadratic contribution is:

   $$\frac{dx^2}{2} \cdot \frac{1}{2}\nabla^2 f = \frac{dx^2}{4}\nabla^2 f.$$

Thus:

$$\langle f \rangle_{\text{around}} \approx f(x_0) + \frac{dx^2}{4}\nabla^2 f(x_0).$$

Rearrange and take the limit:

$$\nabla^2 f(x_0) = \lim_{dx \to 0} 4 \frac{\langle f \rangle_{\text{around}} - f(x_0)}{dx^2}. \tag{4}$$

4 Intuitive Explanation

The Laplacian $\nabla^2 f(x_0)$ measures how the value of f at x_0 compares to its average over an infinitesimal neighborhood:

- If $\nabla^2 f(x_0) > 0$, $f(x_0)$ is less than the neighborhood average, indicating a "valley" (concave-up behavior, like a local minimum).
- If $\nabla^2 f(x_0) < 0$, $f(x_0)$ is greater than the average, indicating a "peak" (concave-down behavior, like a local maximum).
- If $\nabla^2 f(x_0) = 0$, f is harmonic, meaning its value at x_0 equals the neighborhood average.

The factors 4 (2D) and 6 (3D) arise from the geometry of the circle and sphere, respectively, and the dimensionality of the space. This interpretation connects to physical phenomena:

- In **diffusion**, $\nabla^2 f$ describes how a quantity (e.g., heat, concentration) spreads from regions of high to low values.
- In **electrostatics**, Poisson's equation $\nabla^2 \phi = -\rho/\epsilon_0$ relates the Laplacian of the potential to charge density.

5 Examples

5.1 Example 1: 2D, Continuous Form

Consider $f(x, y) = x^2 + y^2$. Compute $\nabla^2 f$:

$$\frac{\partial f}{\partial x} = 2x, \quad \frac{\partial^2 f}{\partial x^2} = 2, \quad \frac{\partial f}{\partial y} = 2y, \quad \frac{\partial^2 f}{\partial y^2} = 2.$$

$$\nabla^2 f = 2 + 2 = 4.$$

This positive Laplacian indicates that f is concave-up, consistent with a paraboloid.

5.2 Example 2: 2D, Discrete Form

For $f(x, y) = x^2 + y^2$ at $x_0 = (0, 0)$, approximate $\langle f\rangle_{\text{around}}$ over a circle of radius dx. Parameterize the circle as $(dx\cos\theta, dx\sin\theta)$:

$$f(dx\cos\theta, dx\sin\theta) = (dx\cos\theta)^2 + (dx\sin\theta)^2 = dx^2(\cos^2\theta + \sin^2\theta) = dx^2.$$

$$\langle f\rangle_{\text{around}} = \frac{1}{2\pi}\int_0^{2\pi} dx^2\, d\theta = dx^2.$$

Since $f(0, 0) = 0$:

$$\nabla^2 f \approx 4\frac{\langle f\rangle_{\text{around}} - f(0, 0)}{dx^2} = 4\frac{dx^2 - 0}{dx^2} = 4.$$

In the limit $dx \to 0$, $\nabla^2 f = 4$, matching the continuous form.

5.3 Example 3: 3D, Continuous Form

Consider $f(x,y,z) = x^2 + y^2 + z^2$. Compute $\nabla^2 f$:

$$\frac{\partial^2 f}{\partial x^2} = 2, \quad \frac{\partial^2 f}{\partial y^2} = 2, \quad \frac{\partial^2 f}{\partial z^2} = 2.$$

$$\nabla^2 f = 2 + 2 + 2 = 6.$$

The positive value reflects the paraboloid's curvature.

5.4 Example 4: 3D, Discrete Form

For $f(x,y,z) = x^2+y^2+z^2$ at $x_0 = (0,0,0)$, approximate $\langle f \rangle_{\text{around}}$ over a sphere of radius dx. Use spherical coordinates $(dx \sin\theta\cos\phi, dx\sin\theta\sin\phi, dx\cos\theta)$:

$$f = (dx\sin\theta\cos\phi)^2 + (dx\sin\theta\sin\phi)^2 + (dx\cos\theta)^2 = dx^2(\sin^2\theta\cos^2\phi + \sin^2\theta\sin^2\phi + \cos^2\theta) = dx^2.$$

$$\langle f \rangle_{\text{around}} = \frac{1}{4\pi}\int_0^{\pi}\int_0^{2\pi} dx^2 \sin\theta \, d\theta \, d\phi = dx^2 \cdot \frac{1}{4\pi} \cdot 4\pi = dx^2.$$

Since $f(0,0,0) = 0$:

$$\nabla^2 f \approx 6\frac{\langle f \rangle_{\text{around}} - f(0,0,0)}{dx^2} = 6\frac{dx^2 - 0}{dx^2} = 6.$$

In the limit, $\nabla^2 f = 6$, matching the continuous form.

5.5 Example 5: 2D Harmonic Function

Consider $f(x,y) = x^2 - y^2$, a harmonic function. Continuous form:

$$\frac{\partial^2 f}{\partial x^2} = 2, \quad \frac{\partial^2 f}{\partial y^2} = -2.$$

$$\nabla^2 f = 2 - 2 = 0.$$

Discrete form at $(0,0)$:

$$f(dx\cos\theta, dx\sin\theta) = dx^2\cos^2\theta - dx^2\sin^2\theta = dx^2(\cos^2\theta - \sin^2\theta).$$

$$\langle f \rangle_{\text{around}} = \frac{1}{2\pi}\int_0^{2\pi} dx^2(\cos^2\theta - \sin^2\theta)\, d\theta = dx^2 \cdot \frac{1}{2\pi} \cdot 0 = 0.$$

$$\nabla^2 f \approx 4\frac{0-0}{dx^2} = 0.$$

The Laplacian is zero, confirming harmonicity.

6 Applications

- **Diffusion**: The heat equation $\frac{\partial u}{\partial t} = \alpha \nabla^2 u$ uses the Laplacian to describe how heat spreads.
- **Electrostatics**: Poisson's equation $\nabla^2 \phi = -\rho/\epsilon_0$ relates the electric potential to charge density.
- **Numerical Methods**: The discrete form inspires finite-difference approximations for solving partial differential equations.
- **Image Processing**: The Laplacian detects edges by highlighting regions of rapid intensity change.

7 Summary

The discrete Laplacian form, derived from averaging over a circle (2D) or sphere (3D), is equivalent to the continuous form. The factors 4 (2D) and 6 (3D) reflect the geometry of the averaging region. The Laplacian measures local curvature, with positive, negative, or zero values indicating valleys, peaks, or harmonic behavior, respectively. Examples confirm consistency between forms, and applications highlight the operator's versatility.

Computing the Laplacian of Functions with Two or Three Variables

May 7, 2025

Abstract

This document presents two methods for computing the Laplacian $\nabla^2 f$ of a scalar function f with two or three variables: (1) direct computation in Cartesian coordinates and (2) transformation to polar or spherical coordinates. Each method is explained with mathematical formulations, practical considerations, and examples. These approaches are fundamental in fields such as physics, engineering, and applied mathematics.

1 Introduction

The Laplacian operator ∇^2 is a second-order differential operator that measures the divergence of the gradient of a scalar function f. For a function f with two or three variables, the Laplacian quantifies how the function changes spatially, making it essential in applications like heat conduction, electrostatics, and fluid dynamics. This document outlines two distinct methods to compute $\nabla^2 f$, highlighting their advantages and use cases.

2 Method 1: Direct Computation in Cartesian Coordinates

The simplest and most straightforward method to compute the Laplacian is to apply the operator directly in Cartesian coordinates.

2.1 Formulation

For a scalar function f:

- In **two dimensions** (x, y), the Laplacian is:

$$\nabla^2 f = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2}$$

- In **three dimensions** (x, y, z), the Laplacian is:

$$\nabla^2 f = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} + \frac{\partial^2 f}{\partial z^2}$$

2.2 Procedure

1. Compute the second partial derivative of f with respect to each variable.
2. Sum the second partial derivatives to obtain $\nabla^2 f$.

2.3 Advantages

- Intuitive and aligns with the standard definition of the Laplacian.
- Requires no coordinate transformation, making it computationally simple for functions defined in Cartesian coordinates.
- Applicable to any differentiable function, regardless of symmetry.

2.4 Example: Two Dimensions

Consider $f(x, y) = x^2 + y^2$.

1. Compute second partial derivatives:

$$\frac{\partial f}{\partial x} = 2x, \quad \frac{\partial^2 f}{\partial x^2} = 2$$
$$\frac{\partial f}{\partial y} = 2y, \quad \frac{\partial^2 f}{\partial y^2} = 2$$

2. Sum the second derivatives:

$$\nabla^2 f = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} = 2 + 2 = 4$$

Result: $\nabla^2 f = 4$.

2.5 Example: Three Dimensions

Consider $f(x, y, z) = x^2 + y^2 + z^2$.

1. Compute second partial derivatives:

$$\frac{\partial f}{\partial x} = 2x, \quad \frac{\partial^2 f}{\partial x^2} = 2$$
$$\frac{\partial f}{\partial y} = 2y, \quad \frac{\partial^2 f}{\partial y^2} = 2$$
$$\frac{\partial f}{\partial z} = 2z, \quad \frac{\partial^2 f}{\partial z^2} = 2$$

2. Sum the second derivatives:

$$\nabla^2 f = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} + \frac{\partial^2 f}{\partial z^2} = 2 + 2 + 2 = 6$$

Result: $\nabla^2 f = 6$.

2.6 Limitations

- May become cumbersome for functions with complex expressions.
- Inefficient for problems with radial or angular symmetry, where polar or spherical coordinates simplify the computation.

3 Method 2: Coordinate Transformation (Polar or Spherical Coordinates)

For functions exhibiting radial or angular symmetry, transforming the function into polar (2D) or spherical (3D) coordinates can simplify the computation of the Laplacian.

3.1 Formulation

The Laplacian operator changes depending on the coordinate system.

3.1.1 Polar Coordinates (2D)

In polar coordinates (r, θ), where $x = r\cos\theta$, $y = r\sin\theta$, the Laplacian of a function $f(r, \theta)$ is:

$$\nabla^2 f = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial f}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 f}{\partial \theta^2} \tag{1}$$

This can be expanded as:

$$\nabla^2 f = \frac{\partial^2 f}{\partial r^2} + \frac{1}{r}\frac{\partial f}{\partial r} + \frac{1}{r^2}\frac{\partial^2 f}{\partial \theta^2}$$

3.1.2 Spherical Coordinates (3D)

In spherical coordinates (r, θ, ϕ), where $x = r\sin\theta\cos\phi$, $y = r\sin\theta\sin\phi$, $z = r\cos\theta$, the Laplacian of a function $f(r, \theta, \phi)$ is:

$$\nabla^2 f = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial f}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta\frac{\partial f}{\partial \theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2 f}{\partial \phi^2} \tag{2}$$

For a radially symmetric function $f(r)$, this simplifies to:

$$\nabla^2 f(r) = \frac{2}{r}\frac{\partial f}{\partial r} + \frac{\partial^2 f}{\partial r^2}$$

3.2 Procedure

1. Express the function f in polar or spherical coordinates by substituting the appropriate coordinate transformations.
2. Compute the partial derivatives as required by the Laplacian formula in the chosen coordinate system.
3. Simplify the expression, leveraging symmetry if applicable.

3.3 Advantages

- Simplifies calculations for functions with radial or angular symmetry (e.g., $f(r)$ in 3D or $f(r, \theta)$ in 2D).
- Reduces the number of terms in problems with spherical or cylindrical symmetry.
- Commonly used in physics for problems like the Coulomb potential or wavefunctions.

3.4 Example: Two Dimensions (Polar Coordinates)

Consider $f(x, y) = x^2 + y^2$. In polar coordinates, $x = r\cos\theta$, $y = r\sin\theta$, so:

$$f(r, \theta) = (r\cos\theta)^2 + (r\sin\theta)^2 = r^2(\cos^2\theta + \sin^2\theta) = r^2$$

Compute the Laplacian:

1. Partial derivatives with respect to r:

$$\frac{\partial f}{\partial r} = \frac{\partial}{\partial r}(r^2) = 2r, \quad \frac{\partial^2 f}{\partial r^2} = 2$$

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial f}{\partial r}\right) = \frac{1}{r}\frac{\partial}{\partial r}(r \cdot 2r) = \frac{1}{r}\frac{\partial}{\partial r}(2r^2) = \frac{1}{r} \cdot 4r = 4$$

2. Partial derivatives with respect to θ:

$$\frac{\partial f}{\partial \theta} = 0, \quad \frac{\partial^2 f}{\partial \theta^2} = 0$$

3. Combine:

$$\nabla^2 f = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial f}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 f}{\partial \theta^2} = 4 + 0 = 4$$

Result: $\nabla^2 f = 4$, matching the Cartesian result.

3.5 Example: Three Dimensions (Spherical Coordinates)

Consider $f(x, y, z) = x^2 + y^2 + z^2$. In spherical coordinates, $r = \sqrt{x^2 + y^2 + z^2}$, so:

$$f(r) = r^2$$

Since f depends only on r, use the simplified Laplacian:

1. Compute derivatives:

$$\frac{\partial f}{\partial r} = 2r, \quad \frac{\partial^2 f}{\partial r^2} = 2$$

2. Apply the formula:

$$\nabla^2 f = \frac{2}{r}\frac{\partial f}{\partial r} + \frac{\partial^2 f}{\partial r^2} = \frac{2}{r}(2r) + 2 = 4 + 2 = 6$$

Result: $\nabla^2 f = 6$, matching the Cartesian result.

3.6 Limitations

- Requires transforming the function into the new coordinate system, which can be complex for non-symmetric functions.
- Singularities (e.g., at $r = 0$ or $\theta = 0, \pi$) may complicate calculations.
- More involved for functions without clear symmetry.

4 Comparison of Methods

Table 1: Comparison of Laplacian Computation Methods

Aspect	**Cartesian**	**Polar/Spherical**
Simplicity	High	Moderate
Best for	General functions	Symmetric functions
Coordinate Transformation	None	Required
Handling Singularities	None	Possible (e.g., $r = 0$)
Computational Effort	Low	Higher for non-symmetric cases

5 Conclusion

The Laplacian of a function with two or three variables can be computed effectively using either direct computation in Cartesian coordinates or transformation to polar/spherical coordinates. The Cartesian method is straightforward and universally applicable, while the coordinate transformation method excels in problems with radial or angular symmetry. The choice of method depends on the function's form and the problem's context, with both approaches yielding consistent results when applied correctly.

Conversion Between Cartesian and Spherical Coordinates

May 7, 2025

Abstract

This document provides a comprehensive guide to converting between Cartesian (x, y, z) and spherical (r, θ, ϕ) coordinate systems. It includes detailed conversion formulas, geometric interpretations, unit vector relationships, and the volume element. Practical examples, common pitfalls, and applications in physics and engineering are discussed. The Laplacian operator in spherical coordinates is derived, and its simplified form for spherically symmetric functions is presented.

1 Introduction

The spherical coordinate system is a powerful tool for describing points in three-dimensional space, particularly in problems exhibiting spherical symmetry, such as those in electromagnetism, quantum mechanics, and astrophysics. Unlike the Cartesian coordinate system, which uses linear distances (x, y, z), the spherical system uses a radial distance r, a polar angle θ, and an azimuthal angle ϕ. This document outlines the conversion between these systems, their geometric relationships, and practical considerations.

2 Spherical Coordinate System

A point in 3D space is represented in spherical coordinates by:

- r: Radial distance from the origin ($0 \leq r < \infty$).
- θ: Polar angle measured from the positive z-axis ($0 \leq \theta \leq \pi$).
- ϕ: Azimuthal angle measured from the positive x-axis in the xy-plane ($0 \leq \phi < 2\pi$).

The geometric interpretation is illustrated in Figure 1.

Figure 1: Spherical coordinate system showing r, θ, and ϕ. (Source: Wikimedia Commons)

3 Conversion Formulas

3.1 Cartesian to Spherical

Given a point (x, y, z) in Cartesian coordinates, the spherical coordinates (r, θ, ϕ) are computed as:

$$\begin{cases} r = \sqrt{x^2 + y^2 + z^2} \\ \theta = \arccos\left(\frac{z}{r}\right) \\ \phi = \arctan\left(\frac{y}{x}\right) \end{cases} \tag{1}$$

Notes:

- The function $\arctan(y/x)$ must account for the quadrant of the point. In programming, use `atan2(y, x)` to handle all cases correctly.
- If $r = 0$, θ and ϕ are undefined (origin).
- If $x = 0$, then $\phi = \pi/2$ (for $y > 0$) or $\phi = 3\pi/2$ (for $y < 0$).

3.2 Spherical to Cartesian

Given spherical coordinates (r, θ, ϕ), the Cartesian coordinates (x, y, z) are:

$$\begin{cases} x = r \sin\theta \cos\phi \\ y = r \sin\theta \sin\phi \\ z = r \cos\theta \end{cases} \tag{2}$$

Geometric Interpretation:

- $r \sin\theta$ is the distance from the z-axis (projection onto the xy-plane).
- $z = r\cos\theta$ represents the height along the z-axis.
- $\cos\phi$ and $\sin\phi$ determine the direction in the xy-plane.

4 Key Relationships

4.1 Unit Vectors

The spherical coordinate unit vectors $\hat{r}$, $\hat{\theta}$, and $\hat{\phi}$ are expressed in terms of Cartesian unit vectors $\hat{x}$, $\hat{y}$, and $\hat{z}$ as:

$$\begin{cases} \hat{r} = \sin\theta\cos\phi\,\hat{x} + \sin\theta\sin\phi\,\hat{y} + \cos\theta\,\hat{z} \\ \hat{\theta} = \cos\theta\cos\phi\,\hat{x} + \cos\theta\sin\phi\,\hat{y} - \sin\theta\,\hat{z} \\ \hat{\phi} = -\sin\phi\,\hat{x} + \cos\phi\,\hat{y} \end{cases} \tag{3}$$

These vectors are orthogonal and form a basis for the spherical coordinate system at each point.

4.2 Volume Element

The differential volume element in spherical coordinates is:

$$dV = r^2 \sin\theta \, dr \, d\theta \, d\phi \tag{4}$$

This accounts for the scaling factors in the radial, polar, and azimuthal directions, making it essential for integrals in spherical coordinates.

5 Laplacian in Spherical Coordinates

The Laplacian operator $\nabla^2 f$ for a scalar function $f(r, \theta, \phi)$ in spherical coordinates is:

$$\nabla^2 f = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial f}{\partial r}\right) + \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta \frac{\partial f}{\partial \theta}\right) + \frac{1}{r^2 \sin^2\theta}\frac{\partial^2 f}{\partial \phi^2} \tag{5}$$

For a spherically symmetric function $f = f(r)$, the Laplacian simplifies to:

$$\nabla^2 f(r) = \frac{1}{r^2}\frac{d}{dr}\left(r^2 \frac{df}{dr}\right) = \frac{2}{r}\frac{df}{dr} + \frac{d^2 f}{dr^2} \tag{6}$$

This form is widely used in problems like solving the Poisson equation or the Schrödinger equation for radial potentials.

6 Examples

6.1 Example 1: Cartesian to Spherical

Convert the point $(1, 1, \sqrt{2})$ to spherical coordinates.

1. Compute r:

$$r = \sqrt{1^2 + 1^2 + (\sqrt{2})^2} = \sqrt{1+1+2} = \sqrt{4} = 2$$

2. Compute θ:

$$\theta = \arccos\left(\frac{\sqrt{2}}{2}\right) = \arccos\left(\frac{\sqrt{2}/\sqrt{2}}{2/\sqrt{2}}\right) = \arccos\left(\frac{1}{\sqrt{2}}\right) = \frac{\pi}{4}$$

3. Compute ϕ:

$$\phi = \arctan\left(\frac{1}{1}\right) = \arctan(1) = \frac{\pi}{4}$$

Result: $(r, \theta, \phi) = \left(2, \frac{\pi}{4}, \frac{\pi}{4}\right)$.

6.2 Example 2: Spherical to Cartesian

Convert the point $\left(2, \frac{\pi}{4}, \frac{\pi}{4}\right)$ to Cartesian coordinates.

1. Compute x:

$$x = 2\sin\left(\frac{\pi}{4}\right)\cos\left(\frac{\pi}{4}\right) = 2 \cdot \frac{\sqrt{2}}{2} \cdot \frac{\sqrt{2}}{2} = 2 \cdot \frac{1}{2} = 1$$

2. Compute y:

$$y = 2\sin\left(\frac{\pi}{4}\right)\sin\left(\frac{\pi}{4}\right) = 2 \cdot \frac{\sqrt{2}}{2} \cdot \frac{\sqrt{2}}{2} = 1$$

3. Compute z:

$$z = 2\cos\left(\frac{\pi}{4}\right) = 2 \cdot \frac{\sqrt{2}}{2} = \sqrt{2}$$

Result: $(x, y, z) = (1, 1, \sqrt{2})$.

7 Common Pitfalls

1. **Angle Conventions**: In physics, θ is often the azimuthal angle and ϕ the polar angle, opposite to the mathematical convention used here. Always verify the convention.

2. **Singularities**: At $\theta = 0$ or $\theta = \pi$ (along the z-axis), ϕ is undefined. At $r = 0$, both θ and ϕ are undefined.

3. **Range of ϕ**: Some texts use $-\pi \leq \phi \leq \pi$ instead of $0 \leq \phi < 2\pi$. Ensure consistency.

4. **Numerical Stability**: When computing ϕ numerically, avoid division by zero by using `atan2`.

8 Applications

Spherical coordinates are indispensable in:

- **Electromagnetism**: Solving for the electric potential of a point charge (Coulomb's law).
- **Quantum Mechanics**: Describing the hydrogen atom's wavefunction.
- **Astrophysics**: Modeling gravitational fields of spherical objects like stars or planets.
- **Computer Graphics**: Rendering 3D objects with spherical symmetry.
- **Fluid Dynamics**: Analyzing flows with radial symmetry.

9 Summary

The conversion between Cartesian and spherical coordinates is summarized in Table 1.

Table 1: Conversion Between Coordinate Systems

Cartesian (x, y, z)	**Spherical** (r, θ, ϕ)
$x = r \sin\theta \cos\phi$	$r = \sqrt{x^2 + y^2 + z^2}$
$y = r \sin\theta \sin\phi$	$\theta = \arccos(z/r)$
$z = r \cos\theta$	$\phi = \arctan(y/x)$

10 Conclusion

Understanding the relationship between Cartesian and spherical coordinates is essential for solving problems in physics, engineering, and computer science. By leveraging the symmetry of spherical coordinates, complex problems can be simplified, and the provided formulas and examples serve as a foundation for practical applications.

Nabla-Laplacian Calculations: Two Methods

Your Name

May 7, 2025

1 Introduction

The Laplacian operator is a second-order differential operator that appears in many areas of physics and mathematics, particularly in electromagnetism, fluid dynamics, and quantum mechanics. It is denoted by the symbol ∇^2 or Δ.

In this document, we'll explore two methods for calculating the Laplacian:

1. Using partial derivatives in Cartesian coordinates
2. Using the spherical method (in spherical coordinates)

2 Method 1: Partial Derivatives in Cartesian Coordinates

In Cartesian coordinates (x, y, z), the Laplacian of a scalar function f is defined as:

$$\nabla^2 f = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} + \frac{\partial^2 f}{\partial z^2}$$

This can be written using the nabla operator ∇ as:

$$\nabla^2 f = \nabla \cdot \nabla f = \nabla \cdot \mathrm{grad}(f)$$

where ∇ is defined as:

$$\nabla = \vec{i}\frac{\partial}{\partial x} + \vec{j}\frac{\partial}{\partial y} + \vec{k}\frac{\partial}{\partial z}$$

2.1 Example 1: Calculate $\nabla^2(x^2 + y^2 + z^2)$

Let's calculate the Laplacian of $f(x, y, z) = x^2 + y^2 + z^2$.

Step 1: Calculate the second partial derivatives.

$$\frac{\partial f}{\partial x} = 2x \quad \Rightarrow \quad \frac{\partial^2 f}{\partial x^2} = 2$$

$$\frac{\partial f}{\partial y} = 2y \quad \Rightarrow \quad \frac{\partial^2 f}{\partial y^2} = 2$$

$$\frac{\partial f}{\partial z} = 2z \quad \Rightarrow \quad \frac{\partial^2 f}{\partial z^2} = 2$$

Step 2: Add the second partial derivatives.

$$\nabla^2 f = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} + \frac{\partial^2 f}{\partial z^2} = 2 + 2 + 2 = 6$$

Therefore, $\nabla^2(x^2 + y^2 + z^2) = 6$.

2.2 Example 2: Calculate $\nabla^2(xyz)$

Let's calculate the Laplacian of $f(x, y, z) = xyz$.

Step 1: Calculate the second partial derivatives.

$$\frac{\partial f}{\partial x} = yz \quad \Rightarrow \quad \frac{\partial^2 f}{\partial x^2} = 0$$

$$\frac{\partial f}{\partial y} = xz \quad \Rightarrow \quad \frac{\partial^2 f}{\partial y^2} = 0$$

$$\frac{\partial f}{\partial z} = xy \quad \Rightarrow \quad \frac{\partial^2 f}{\partial z^2} = 0$$

Step 2: Add the second partial derivatives.

$$\nabla^2 f = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} + \frac{\partial^2 f}{\partial z^2} = 0 + 0 + 0 = 0$$

Therefore, $\nabla^2(xyz) = 0$.

3 Method 2: Spherical Method

In spherical coordinates (r, θ, ϕ), the Laplacian takes a different form:

$$\nabla^2 f = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial f}{\partial r}\right) + \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta \frac{\partial f}{\partial \theta}\right) + \frac{1}{r^2 \sin^2\theta}\frac{\partial^2 f}{\partial \phi^2}$$

For functions that depend only on the radial distance r (spherically symmetric functions), this simplifies to:

$$\nabla^2 f(r) = \frac{1}{r^2}\frac{d}{dr}\left(r^2 \frac{df}{dr}\right) = \frac{1}{r^2}\frac{d}{dr}\left(r^2 f'\right) = f'' + \frac{2}{r} f'$$

3.1 Example 3: Calculate $\nabla^2(1/r)$ in spherical coordinates

Let's calculate the Laplacian of $f(r) = \frac{1}{r}$ using the spherical method.

Step 1: Find the first derivative with respect to r.

$$f'(r) = \frac{d}{dr}\left(\frac{1}{r}\right) = -\frac{1}{r^2}$$

Step 2: Find the second derivative with respect to r.

$$f''(r) = \frac{d}{dr}\left(-\frac{1}{r^2}\right) = \frac{2}{r^3}$$

Step 3: Apply the spherical Laplacian formula for radially symmetric functions.

$$\nabla^2 f(r) = f''(r) + \frac{2}{r}f'(r) = \frac{2}{r^3} + \frac{2}{r}\left(-\frac{1}{r^2}\right) = \frac{2}{r^3} - \frac{2}{r^3} = 0$$

Therefore, $\nabla^2(1/r) = 0$ for $r \neq 0$.

This is a very important result in physics! The function $1/r$ represents the Coulomb potential in electrostatics and the gravitational potential for point masses. The fact that its Laplacian is zero outside the origin tells us it satisfies Laplace's equation in free space.

3.2 Example 4: Calculate $\nabla^2(r^2)$ in spherical coordinates

Let's calculate the Laplacian of $f(r) = r^2$ using the spherical method.

Step 1: Find the first derivative with respect to r.

$$f'(r) = \frac{d}{dr}(r^2) = 2r$$

Step 2: Find the second derivative with respect to r.

$$f''(r) = \frac{d}{dr}(2r) = 2$$

Step 3: Apply the spherical Laplacian formula for radially symmetric functions.

$$\nabla^2 f(r) = f''(r) + \frac{2}{r}f'(r) = 2 + \frac{2}{r}(2r) = 2 + 4 = 6$$

Therefore, $\nabla^2(r^2) = 6$.

Note that this matches our result from Example 1 since $r^2 = x^2 + y^2 + z^2$ in Cartesian coordinates. This confirms the consistency between the two methods.

4 Relationship Between the Two Methods

The two methods for calculating the Laplacian are equivalent and will always give the same result for the same function. The choice of which method to use depends on the coordinate system that best suits the problem and the symmetry of the function.

For functions with spherical symmetry (i.e., functions that depend only on r), the spherical method is usually simpler. For functions expressed in Cartesian coordinates without obvious symmetry, the partial derivatives method is typically more straightforward.

5 Practical Applications

The Laplacian operator appears in many important equations in physics:

1. **Poisson's equation**: $\nabla^2\phi = -\rho/\epsilon_0$ (electrostatics)
2. **Heat equation**: $\frac{\partial T}{\partial t} = \alpha\nabla^2 T$ (heat transfer)
3. **Wave equation**: $\frac{\partial^2 u}{\partial t^2} = c^2\nabla^2 u$ (acoustics, electromagnetism)
4. **Schrödinger equation**: $i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + V\psi$ (quantum mechanics)

Understanding how to calculate the Laplacian is therefore essential in many areas of physics and engineering.

Saddle Points and the Hessian Matrix: Extended Examples

1 Introduction

A saddle point is a critical point of a function where the function behaves like a saddle - rising in some directions and falling in others. The Hessian matrix provides a powerful tool for identifying and analyzing saddle points.

2 The Hessian Matrix and Its Determinant

For a function $f(x, y, z)$, the Hessian matrix at a point p is the square matrix of all second-order partial derivatives:

$$H(f) = \begin{bmatrix} \frac{\partial^2 f}{\partial x^2} & \frac{\partial^2 f}{\partial x \partial y} & \frac{\partial^2 f}{\partial x \partial z} \\ \frac{\partial^2 f}{\partial y \partial x} & \frac{\partial^2 f}{\partial y^2} & \frac{\partial^2 f}{\partial y \partial z} \\ \frac{\partial^2 f}{\partial z \partial x} & \frac{\partial^2 f}{\partial z \partial y} & \frac{\partial^2 f}{\partial z^2} \end{bmatrix}$$

For a critical point (x_0, y_0) of a function $f(x, y)$, the determinant of the Hessian helps classify the nature of the point:

$$\det(H) = \frac{\partial^2 f}{\partial x^2} \cdot \frac{\partial^2 f}{\partial y^2} - \left(\frac{\partial^2 f}{\partial x \partial y}\right)^2$$

- If $\det(H) > 0$ and $\frac{\partial^2 f}{\partial x^2} > 0$, the point is a local minimum
- If $\det(H) > 0$ and $\frac{\partial^2 f}{\partial x^2} < 0$, the point is a local maximum
- If $\det(H) < 0$, the point is a saddle point
- If $\det(H) = 0$, the test is inconclusive, and higher-order derivatives must be examined

3 Examples of Saddle Points in Two Variables

3.1 Example 1: Classic Hyperbolic Paraboloid $f(x, y) = x^2 - y^2$

First derivatives:

$$\frac{\partial f}{\partial x} = 2x$$
$$\frac{\partial f}{\partial y} = -2y$$

Critical point: $(0, 0)$ where both partial derivatives equal zero.
Second derivatives:

$$\frac{\partial^2 f}{\partial x^2} = 2$$
$$\frac{\partial^2 f}{\partial y^2} = -2$$
$$\frac{\partial^2 f}{\partial x \partial y} = 0$$

Hessian matrix:

$$H(f) = \begin{bmatrix} 2 & 0 \\ 0 & -2 \end{bmatrix}$$

Determinant:

$$\det(H) = 2 \times (-2) - 0 \times 0 = -4 < 0$$

Eigenvalues: $\lambda_1 = 2 > 0$, $\lambda_2 = -2 < 0$
Conclusion: The point $(0, 0)$ is a saddle point, with the function increasing in the x direction and decreasing in the y direction.

3.2 Example 2: Cross-Product Function $f(x, y) = xy$

First derivatives:

$$\frac{\partial f}{\partial x} = y$$
$$\frac{\partial f}{\partial y} = x$$

Critical point: $(0, 0)$ where both partial derivatives equal zero.
Second derivatives:

$$\frac{\partial^2 f}{\partial x^2} = 0$$
$$\frac{\partial^2 f}{\partial y^2} = 0$$
$$\frac{\partial^2 f}{\partial x \partial y} = 1$$

Hessian matrix:
$$H(f) = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

Determinant:
$$\det(H) = 0 \times 0 - 1 \times 1 = -1 < 0$$

Eigenvalues: $\lambda_1 = 1 > 0$, $\lambda_2 = -1 < 0$

Conclusion: The point $(0, 0)$ is a saddle point. The function increases along the line $y = x$ and decreases along the line $y = -x$.

3.3 Example 3: Cubic Function $f(x, y) = x^3 + y^3 - 3xy$

First derivatives:

$$\frac{\partial f}{\partial x} = 3x^2 - 3y$$
$$\frac{\partial f}{\partial y} = 3y^2 - 3x$$

Setting these equal to zero and solving the system:

$$x^2 = y$$
$$y^2 = x$$

Substituting the first equation into the second:

$$(x^2)^2 = x$$
$$x^4 = x$$
$$x^4 - x = 0$$
$$x(x^3 - 1) = 0$$

This gives $x = 0$ or $x = 1$. When $x = 0$, $y = 0$. When $x = 1$, $y = 1$.

Critical points: $(0, 0)$ and $(1, 1)$

Second derivatives:

$$\frac{\partial^2 f}{\partial x^2} = 6x$$
$$\frac{\partial^2 f}{\partial y^2} = 6y$$
$$\frac{\partial^2 f}{\partial x \partial y} = -3$$

For critical point $(0, 0)$:

$$H(f)_{(0,0)} = \begin{bmatrix} 0 & -3 \\ -3 & 0 \end{bmatrix}$$

Determinant:

$$\det(H)_{(0,0)} = 0 \times 0 - (-3) \times (-3) = -9 < 0$$

Eigenvalues: $\lambda_1 = 3 > 0$, $\lambda_2 = -3 < 0$
Conclusion: The point $(0, 0)$ is a saddle point.
For critical point $(1, 1)$:

$$H(f)_{(1,1)} = \begin{bmatrix} 6 & -3 \\ -3 & 6 \end{bmatrix}$$

Determinant:

$$\det(H)_{(1,1)} = 6 \times 6 - (-3) \times (-3) = 36 - 9 = 27 > 0$$

Since $\det(H) > 0$ and $\frac{\partial^2 f}{\partial x^2} = 6 > 0$, the point $(1, 1)$ is a local minimum.

3.4 Example 4: Monkey Saddle $f(x, y) = x^3 - 3xy^2$

The "monkey saddle" is named because it has three "depressions" (like a saddle with a place for a monkey's tail).

First derivatives:

$$\frac{\partial f}{\partial x} = 3x^2 - 3y^2$$
$$\frac{\partial f}{\partial y} = -6xy$$

Critical point: Setting both equal to zero: $3x^2 - 3y^2 = 0$ implies $x^2 = y^2$, so $x = \pm y$. $-6xy = 0$ implies either $x = 0$ or $y = 0$.

If $x = 0$, then $y^2 = 0$, so $y = 0$. If $y = 0$, then $x^2 = 0$, so $x = 0$.

This gives us the critical point $(0, 0)$.

Second derivatives:

$$\frac{\partial^2 f}{\partial x^2} = 6x$$
$$\frac{\partial^2 f}{\partial y^2} = -6x$$
$$\frac{\partial^2 f}{\partial x \partial y} = -6y$$

Hessian at $(0, 0)$:

$$H(f)_{(0,0)} = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}$$

Determinant: $\det(H) = 0 \times 0 - 0 \times 0 = 0$

Since the determinant is zero, the second-derivative test is inconclusive. However, by examining the function's behavior along different paths, we can determine it's a higher-order saddle point:

- Along the positive x-axis: $f(x, 0) = x^3$ increases
- Along the negative x-axis: $f(x, 0) = x^3$ decreases
- Along the y-axis: $f(0, y) = 0$ remains constant
- Along the lines $y = \pm x$: $f(x, \pm x) = x^3 - 3x \cdot (\pm x)^2 = x^3 - 3x^3 = -2x^3$, which decreases for positive x and increases for negative x

This shows the function has a more complex saddle point structure than the standard saddle point.

4 Examples in Three Variables

4.1 Example 5: $f(x, y, z) = x^2 + y^2 - z^2$

First derivatives:

$$\frac{\partial f}{\partial x} = 2x$$
$$\frac{\partial f}{\partial y} = 2y$$
$$\frac{\partial f}{\partial z} = -2z$$

Critical point: $(0, 0, 0)$

Second derivatives:

$$\frac{\partial^2 f}{\partial x^2} = 2$$
$$\frac{\partial^2 f}{\partial y^2} = 2$$
$$\frac{\partial^2 f}{\partial z^2} = -2$$
$$\frac{\partial^2 f}{\partial x \partial y} = \frac{\partial^2 f}{\partial x \partial z} = \frac{\partial^2 f}{\partial y \partial z} = 0$$

Hessian matrix:

$$H(f) = \begin{bmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & -2 \end{bmatrix}$$

Eigenvalues: $\lambda_1 = 2$, $\lambda_2 = 2$, $\lambda_3 = -2$

With mixed signs of eigenvalues, this is a saddle point. Specifically, it's a first-order saddle point because there is exactly one negative eigenvalue.

Determinant: $\det(H) = 2 \times 2 \times (-2) = -8 < 0$

Note that for a 3×3 matrix, a negative determinant doesn't always guarantee a saddle point (unlike in the 2×2 case). However, in this case, we confirmed it is a saddle point by examining the eigenvalues directly.

4.2 Example 6: $f(x, y, z) = xyz$

First derivatives:

$$\frac{\partial f}{\partial x} = yz$$
$$\frac{\partial f}{\partial y} = xz$$
$$\frac{\partial f}{\partial z} = xy$$

Critical points: Setting all equal to zero:

$$yz = 0$$
$$xz = 0$$
$$xy = 0$$

This is satisfied when at least two of the variables are zero. So the critical points are all points on the coordinate axes, excluding the origin.

For the origin $(0, 0, 0)$, let's calculate the Hessian:

Second derivatives:

$$\frac{\partial^2 f}{\partial x^2} = 0$$
$$\frac{\partial^2 f}{\partial y^2} = 0$$
$$\frac{\partial^2 f}{\partial z^2} = 0$$
$$\frac{\partial^2 f}{\partial x \partial y} = z$$
$$\frac{\partial^2 f}{\partial x \partial z} = y$$
$$\frac{\partial^2 f}{\partial y \partial z} = x$$

At $(0, 0, 0)$, all second derivatives equal zero, giving us a zero Hessian matrix:

$$H(f)_{(0,0,0)} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

Determinant: $\det(H) = 0$

Eigenvalues: $\lambda_1 = \lambda_2 = \lambda_3 = 0$

This is a degenerate critical point, and the second-derivative test is inconclusive.

5 Example 7: Non-obvious Saddle Point $f(x, y) = e^x \sin(y)$

First derivatives:

$$\frac{\partial f}{\partial x} = e^x \sin(y)$$
$$\frac{\partial f}{\partial y} = e^x \cos(y)$$

Critical points: Setting both equal to zero: $e^x \sin(y) = 0$ implies $\sin(y) = 0$ since $e^x > 0$ for all x. $e^x \cos(y) = 0$ implies $\cos(y) = 0$ since $e^x > 0$ for all x.

But $\sin(y)$ and $\cos(y)$ can't both be zero for the same y, so there are no critical points.

However, if we modify the function slightly to $f(x, y) = e^x(\sin(y) - 1)$, then:

$$\frac{\partial f}{\partial x} = e^x(\sin(y) - 1)$$
$$\frac{\partial f}{\partial y} = e^x \cos(y)$$

Critical points: Setting both equal to zero: $e^x(\sin(y) - 1) = 0$ implies $\sin(y) = 1$ since $e^x > 0$. $e^x \cos(y) = 0$ implies $\cos(y) = 0$.

When $\sin(y) = 1$, we have $y = \frac{\pi}{2} + 2n\pi$ where n is an integer, and at these values, $\cos(y) = 0$.

So critical points are $(x, \frac{\pi}{2} + 2n\pi)$ for any real x and integer n.

Let's examine the point $(0, \frac{\pi}{2})$:

Second derivatives:

$$\frac{\partial^2 f}{\partial x^2} = e^x(\sin(y) - 1)$$
$$\frac{\partial^2 f}{\partial y^2} = -e^x \sin(y)$$
$$\frac{\partial^2 f}{\partial x \partial y} = e^x \cos(y)$$

At $(0, \frac{\pi}{2})$:

$$\frac{\partial^2 f}{\partial x^2} = e^0(\sin(\frac{\pi}{2}) - 1) = 1 \times (1 - 1) = 0$$
$$\frac{\partial^2 f}{\partial y^2} = -e^0 \sin(\frac{\pi}{2}) = -1 \times 1 = -1$$
$$\frac{\partial^2 f}{\partial x \partial y} = e^0 \cos(\frac{\pi}{2}) = 1 \times 0 = 0$$

Hessian:

$$H(f) = \begin{bmatrix} 0 & 0 \\ 0 & -1 \end{bmatrix}$$

Determinant: $\det(H) = 0 \times (-1) - 0 \times 0 = 0$
Since the determinant is zero, the second-derivative test is inconclusive.
However, by examining the function's behavior:

- Along the x-axis at $y = \frac{\pi}{2}$: $f(x, \frac{\pi}{2}) = e^x(1-1) = 0$, which is constant.
- Deviating from $y = \frac{\pi}{2}$: $\sin(y) < 1$, making $f(x, y) < 0$ for any x.

This shows $(0, \frac{\pi}{2})$ is a degenerate critical point with saddle-like behavior.

6 Applications and Significance

Saddle points play crucial roles in various fields:

- **Optimization**: Gradient-based methods may slow down or get stuck near saddle points.
- **Physical Chemistry**: First-order saddle points on potential energy surfaces represent transition states between reactants and products.
- **Differential Games**: Saddle points correspond to Nash equilibria in certain games.
- **Machine Learning**: Deep neural networks' loss landscapes contain numerous saddle points rather than local minima.

6.1 Saddle Points in Machine Learning

In high-dimensional spaces (like neural network parameter spaces), saddle points are far more common than local minima. This is because:

- A local minimum requires all eigenvalues to be positive
- A saddle point only requires some negative and some positive eigenvalues
- As dimensionality increases, the probability of all eigenvalues being positive decreases exponentially

In a random matrix with entries drawn from a normal distribution, the probability of all eigenvalues being positive is approximately 2^{-n}, where n is the dimension.

7 Conclusion

The Hessian matrix and its determinant provide powerful tools for identifying and classifying critical points, particularly saddle points. While in two dimensions a negative Hessian determinant is a sufficient condition for a saddle point, in higher dimensions we must examine the eigenvalues directly. The examples presented showcase the variety of saddle point structures that can occur in different functions, from standard saddle points to monkey saddles and degenerate cases.

Saddle Points and the Hessian Matrix

1 Introduction

A saddle point is a critical point of a function where the function behaves like a saddle - rising in some directions and falling in others. The Hessian matrix provides a powerful tool for identifying and analyzing saddle points.

2 The Hessian Matrix

For a function $f(x, y, z)$, the Hessian matrix at a point p is the square matrix of all second-order partial derivatives:

$$H(f) = \begin{bmatrix} \frac{\partial^2 f}{\partial x^2} & \frac{\partial^2 f}{\partial x \partial y} & \frac{\partial^2 f}{\partial x \partial z} \\ \frac{\partial^2 f}{\partial y \partial x} & \frac{\partial^2 f}{\partial y^2} & \frac{\partial^2 f}{\partial y \partial z} \\ \frac{\partial^2 f}{\partial z \partial x} & \frac{\partial^2 f}{\partial z \partial y} & \frac{\partial^2 f}{\partial z^2} \end{bmatrix}$$

3 The Determinant of the Hessian

The determinant of the Hessian matrix provides valuable information about the nature of critical points:

- For a function $f(x, y)$ with a 2×2 Hessian:
  - If $\det(H) > 0$ and $\frac{\partial^2 f}{\partial x^2} > 0$, then the critical point is a local minimum.
  - If $\det(H) > 0$ and $\frac{\partial^2 f}{\partial x^2} < 0$, then the critical point is a local maximum.
  - If $\det(H) < 0$, then the critical point is a saddle point.
- For higher-dimensional functions, we need to examine the sequence of leading principal minors (determinants of upper-left submatrices) of the Hessian.

The determinant is negative at a saddle point (in the two-variable case) because the eigenvalues have mixed signs, and the determinant is the product of all eigenvalues.

4 Saddle Point Characterization

At a critical point (where all first derivatives are zero), the Hessian matrix characterizes the nature of that point:

1. **Positive definite Hessian**: All eigenvalues are positive $\rightarrow$ Local minimum
2. **Negative definite Hessian**: All eigenvalues are negative $\rightarrow$ Local maximum
3. **Indefinite Hessian**: Some eigenvalues are positive and some are negative $\rightarrow$ Saddle point

5 Simplified Case: $f(x, y)$

For a function of two variables, the Hessian is a 2×2 matrix:

$$H(f) = \begin{bmatrix} \frac{\partial^2 f}{\partial x^2} & \frac{\partial^2 f}{\partial x \partial y} \\ \frac{\partial^2 f}{\partial y \partial x} & \frac{\partial^2 f}{\partial y^2} \end{bmatrix}$$

The determinant is calculated as:

$$\det(H) = \frac{\partial^2 f}{\partial x^2} \cdot \frac{\partial^2 f}{\partial y^2} - \frac{\partial^2 f}{\partial x \partial y} \cdot \frac{\partial^2 f}{\partial y \partial x}$$

When the mixed partials are equal (which is usually the case for smooth functions), this simplifies to:

$$\det(H) = \frac{\partial^2 f}{\partial x^2} \cdot \frac{\partial^2 f}{\partial y^2} - \left(\frac{\partial^2 f}{\partial x \partial y} \right)^2$$

6 Classic Example: $f(x, y) = x^2 - y^2$

This is the canonical example of a function with a saddle point at the origin $(0, 0)$.

First derivatives:

$$\frac{\partial f}{\partial x} = 2x$$
$$\frac{\partial f}{\partial y} = -2y$$

At $(0, 0)$, both derivatives are zero, confirming it's a critical point.

The Hessian matrix is:

$$H(f) = \begin{bmatrix} \frac{\partial^2 f}{\partial x^2} & \frac{\partial^2 f}{\partial x \partial y} \\ \frac{\partial^2 f}{\partial y \partial x} & \frac{\partial^2 f}{\partial y^2} \end{bmatrix} = \begin{bmatrix} 2 & 0 \\ 0 & -2 \end{bmatrix}$$

The determinant is:

$$\det(H) = 2 \times (-2) - 0 \times 0 = -4 < 0$$

Since the determinant is negative, this confirms it's a saddle point.
Looking at the eigenvalues of H:

$$\lambda_1 = 2 \text{ (positive)}$$
$$\lambda_2 = -2 \text{ (negative)}$$

The mixed sign of eigenvalues also confirms this is a saddle point.

7 Another Example: $f(x, y) = xy$

For $f(x, y) = xy$, the first derivatives are:

$$\frac{\partial f}{\partial x} = y$$
$$\frac{\partial f}{\partial y} = x$$

At $(0, 0)$, both derivatives are zero, indicating a critical point.
The Hessian matrix is:

$$H(f) = \begin{bmatrix} \frac{\partial^2 f}{\partial x^2} & \frac{\partial^2 f}{\partial x \partial y} \\ \frac{\partial^2 f}{\partial y \partial x} & \frac{\partial^2 f}{\partial y^2} \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

The determinant is:

$$\det(H) = 0 \times 0 - 1 \times 1 = -1 < 0$$

Again, the negative determinant confirms this is a saddle point.
The eigenvalues are $\lambda_1 = 1$ and $\lambda_2 = -1$, showing mixed signs.

8 Three-Variable Example: $f(x, y, z) = x^2 + y^2 - z^2$

For this function, the critical point is at $(0, 0, 0)$. The Hessian is:

$$H(f) = \begin{bmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & -2 \end{bmatrix}$$

The determinant is:

$$\det(H) = 2 \times 2 \times (-2) = -8 < 0$$

While a negative determinant in a 2×2 Hessian always indicates a saddle point, for higher dimensions this is not sufficient. We need to analyze the eigenvalues directly or examine the sequence of principal minors.

For this example, the eigenvalues are $\lambda_1 = 2$, $\lambda_2 = 2$, and $\lambda_3 = -2$, confirming it's a saddle point.

9 Geometric Interpretation

Near a saddle point, the function:

- Increases when moving in directions corresponding to positive eigenvalues
- Decreases when moving in directions corresponding to negative eigenvalues

For our example $f(x, y) = x^2 - y^2$:

- Moving along the x-axis: $f(x, 0) = x^2$ increases as we move away from origin
- Moving along the y-axis: $f(0, y) = -y^2$ decreases as we move away from origin

The surface resembles a horse saddle, rising in one direction while falling in another.

10 Higher Dimensions

In higher dimensions, a critical point is a saddle point if the Hessian has at least one positive and at least one negative eigenvalue.

For a function $f(x_1, x_2, \ldots, x_n)$, there are different "orders" of saddle points based on the number of negative eigenvalues:

- First-order saddle: Exactly one negative eigenvalue
- Second-order saddle: Exactly two negative eigenvalues
- And so on...

11 Applications

Saddle points are important in many fields:

- **Optimization**: They represent challenges for gradient-based methods
- **Quantum chemistry**: First-order saddle points correspond to transition states
- **Machine learning**: Neural network loss functions often have many saddle points
- **Dynamical systems**: Unstable equilibrium points often exhibit saddle-point behavior

12 Conclusion

The Hessian matrix provides a powerful tool for identifying and characterizing saddle points in multivariate functions. The determinant of the Hessian, along with its eigenvalues, gives us clear criteria for distinguishing between different types of critical points. By examining these properties, we can determine not only if a critical point is a saddle point, but also understand how the function behaves in different directions around that point.

Laplacian and Hessian: An Intuitive Connection

Let me explain the connection between the Laplacian operator and the Hessian matrix, with focus on their physical intuition and relationship.

1 The Hessian Matrix

The Hessian matrix contains all second-order partial derivatives of a function. For a function $f(x, y, z)$, the Hessian is:

$$H(f) = \begin{bmatrix} \frac{\partial^2 f}{\partial x^2} & \frac{\partial^2 f}{\partial x \partial y} & \frac{\partial^2 f}{\partial x \partial z} \\ \frac{\partial^2 f}{\partial y \partial x} & \frac{\partial^2 f}{\partial y^2} & \frac{\partial^2 f}{\partial y \partial z} \\ \frac{\partial^2 f}{\partial z \partial x} & \frac{\partial^2 f}{\partial z \partial y} & \frac{\partial^2 f}{\partial z^2} \end{bmatrix}$$

The Hessian tells us about the *curvature* of the function in different directions.

2 The Laplacian Operator

The Laplacian operator is the sum of all unmixed second derivatives:

$$\nabla^2 f = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} + \frac{\partial^2 f}{\partial z^2}$$

3 The Connection

The key connection is: **The Laplacian is the trace of the Hessian matrix**.

$$\nabla^2 f = \mathrm{Tr}(H(f))$$

The trace of a matrix is the sum of its diagonal elements, which in this case are the unmixed second derivatives.

4 Physical Meaning of the Trace

The trace of the Hessian represents the *average curvature* of the function in all coordinate directions. It tells us how the function curves on average around a point.

- Positive trace: The function curves upward on average (like a bowl)
- Negative trace: The function curves downward on average (like an upside-down bowl)
- Zero trace: The curving up in some directions is exactly balanced by curving down in others

5 Simple Examples

5.1 One Variable: $f(x)$

- Hessian: $H(f) = \left[\frac{d^2 f}{dx^2}\right]$ (just a single number)
- Laplacian: $\nabla^2 f = \frac{d^2 f}{dx^2}$
- Example: $f(x) = x^2$
  - $H(f) = [2]$
  - $\nabla^2 f = 2$
  - Physical meaning: The function curves upward everywhere with constant curvature of 2

5.2 Two Variables: $f(x, y)$

- Hessian: $H(f) = \begin{bmatrix} \frac{\partial^2 f}{\partial x^2} & \frac{\partial^2 f}{\partial x \partial y} \\ \frac{\partial^2 f}{\partial y \partial x} & \frac{\partial^2 f}{\partial y^2} \end{bmatrix}$
- Laplacian: $\nabla^2 f = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2}$
- Example: $f(x, y) = x^2 + 3y^2$
  - $H(f) = \begin{bmatrix} 2 & 0 \\ 0 & 6 \end{bmatrix}$
  - $\nabla^2 f = 2 + 6 = 8$
  - Physical meaning: The function curves twice as much in the x direction as a standard parabola, and six times as much in the y direction. The average curvature is 8.

5.3 Three Variables: $f(x, y, z)$

- Hessian: As shown earlier, a 3×3 matrix
- Laplacian: $\nabla^2 f = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} + \frac{\partial^2 f}{\partial z^2}$
- Example: $f(x, y, z) = x^2 - y^2 + z^2$

- $H(f) = \begin{bmatrix} 2 & 0 & 0 \\ 0 & -2 & 0 \\ 0 & 0 & 2 \end{bmatrix}$
- $\nabla^2 f = 2 + (-2) + 2 = 2$
- Physical meaning: The function curves upward in x and z directions, but downward in the y direction. The average curvature is still positive (2), indicating that on average, the function curves upward.

6 Applications

In physics, the Laplacian appears in many equations:

- In potential theory: $\nabla^2 \phi = 0$ (Laplace's equation)
- In heat flow: $\nabla^2 T \propto \frac{\partial T}{\partial t}$ (Heat equation)
- In quantum mechanics: $\nabla^2 \psi \propto \frac{\partial^2 \psi}{\partial t^2}$ (Schrödinger equation)

In all these cases, the Laplacian represents how much a quantity (potential, temperature, probability) at a point differs from the average of its surroundings.

Connection Between the Laplacian and Hessian

The Laplacian and Hessian are both fundamental differential operators in multivariable calculus, with important connections in analysis, physics, and geometry.

Definitions

Hessian Matrix For a twice differentiable function $f : \mathbb{R}^n \to \mathbb{R}$, the Hessian is the matrix of second-order partial derivatives:

$$H(f) = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} & \cdots & \frac{\partial^2 f}{\partial x_2 \partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_n \partial x_1} & \frac{\partial^2 f}{\partial x_n \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_n^2} \end{bmatrix}$$

Laplacian Operator The Laplacian Δ is the trace of the Hessian matrix:

$$\Delta f = \operatorname{tr}(H(f)) = \sum_{i=1}^{n} \frac{\partial^2 f}{\partial x_i^2}$$

Key Connections

1. Trace Relationship The Laplacian is exactly the trace of the Hessian matrix:

$$\Delta f = \operatorname{tr}(H(f)) = \boldsymbol{\nabla} \cdot (\nabla f)$$

This shows the Laplacian measures the *divergence* of the gradient field.

2. Decomposition in $\mathbb{R}^3$ The Hessian can be decomposed into Laplacian and anisotropic components:

$$H(f) = \underbrace{\frac{1}{3}(\Delta f)I}_{\text{Isotropic part}} + \underbrace{\left(H(f) - \frac{1}{3}(\Delta f)I\right)}_{\text{Anisotropic part}}$$

3. Harmonic Functions A function is *harmonic* if its Laplacian vanishes everywhere:

$$\Delta f = 0 \iff \operatorname{tr}(H(f)) = 0$$

This implies the Hessian must be traceless for harmonic functions.

Geometric Interpretation

- **Hessian**: Encodes all second-order derivative information, including directional curvature
- **Laplacian**: Represents the average curvature in all directions (trace)

For $f : \mathbb{R}^2 \to \mathbb{R}$:

$$\Delta f = \kappa_1 + \kappa_2$$

where κ_i are the principal curvatures (eigenvalues of the Hessian).

Example Calculations

Example 1: Quadratic Function Let $f(x, y) = ax^2 + bxy + cy^2$:

$$H(f) = \begin{bmatrix} 2a & b \\ b & 2c \end{bmatrix}, \quad \Delta f = 2a + 2c$$

Example 2: Radial Function For $f(\boldsymbol{x}) = \|\boldsymbol{x}\|^2 = x_1^2 + \cdots + x_n^2$:

$$H(f) = 2I_n, \quad \Delta f = 2n$$

Applications

1. Physics (Wave Equation) The wave equation uses both operators:

$$\frac{\partial^2 u}{\partial t^2} = c^2 \Delta u = c^2 \operatorname{tr}(H(u))$$

2. Machine Learning In optimization, the relationship appears in:

$$\Delta f = \operatorname{tr}(H(f)) = \sum \lambda_i$$

where λ_i are Hessian eigenvalues governing convergence.

3. Image Processing The Laplacian of Gaussian (LoG) operator combines both:

$$LoG(f) = \Delta(G_\sigma * f) = \operatorname{tr}(H(G_\sigma * f))$$

Important Theorems

Bochner's Formula Relates the Laplacian of energy densities to the Hessian:

$$\Delta \left(\frac{1}{2} |\nabla f|^2 \right) = \|H(f)\|_F^2 + \langle \nabla f, \nabla \Delta f \rangle$$

where $\| \cdot \|_F$ is the Frobenius norm.

Maximum Principle For harmonic functions ($\Delta f = 0$), the Hessian must satisfy:

$$\det(H(f)) \leq \left(\frac{\mathrm{tr}(H(f))}{n}\right)^n = 0$$

Corrected Hessian Matrix in Taylor Expansion with Verified Examples

The second-order Taylor expansion for a twice continuously differentiable function $f : \mathbb{R}^n \to \mathbb{R}$ at point $\boldsymbol{a}$ is:

$$f(\boldsymbol{x}) = f(\boldsymbol{a}) + \nabla f(\boldsymbol{a})^\top (\boldsymbol{x} - \boldsymbol{a}) + \frac{1}{2}(\boldsymbol{x} - \boldsymbol{a})^\top H_f(\boldsymbol{a})(\boldsymbol{x} - \boldsymbol{a}) + R_2(\boldsymbol{x}, \boldsymbol{a})$$

where:

- $\nabla f(\boldsymbol{a})$ is the gradient vector at $\boldsymbol{a}$
- $H_f(\boldsymbol{a})$ is the Hessian matrix at $\boldsymbol{a}$
- $R_2(\boldsymbol{x}, \boldsymbol{a})$ is the remainder term (Peano or Lagrange form)

Example 1: Quadratic Polynomial (Corrected)

Consider $f(x, y) = 3x^2 + 2xy + y^2$ at $\boldsymbol{a} = (1, 2)$.

First derivatives:

$$\frac{\partial f}{\partial x} = 6x + 2y, \quad \frac{\partial f}{\partial y} = 2x + 2y$$

$$\nabla f(1, 2) = \begin{pmatrix} 6(1) + 2(2) \\ 2(1) + 2(2) \end{pmatrix} = \begin{pmatrix} 10 \\ 6 \end{pmatrix}$$

Hessian matrix (constant for quadratic forms):

$$H_f = \begin{bmatrix} \frac{\partial^2 f}{\partial x^2} & \frac{\partial^2 f}{\partial x \partial y} \\ \frac{\partial^2 f}{\partial y \partial x} & \frac{\partial^2 f}{\partial y^2} \end{bmatrix} = \begin{bmatrix} 6 & 2 \\ 2 & 2 \end{bmatrix}$$

Taylor expansion (verified):

$$\begin{aligned} f(x, y) &\approx f(1, 2) + \nabla f(1, 2)^\top \begin{pmatrix} x - 1 \\ y - 2 \end{pmatrix} + \frac{1}{2} \begin{pmatrix} x - 1 & y - 2 \end{pmatrix} H_f \begin{pmatrix} x - 1 \\ y - 2 \end{pmatrix} \\ &= 11 + \begin{pmatrix} 10 & 6 \end{pmatrix} \begin{pmatrix} x - 1 \\ y - 2 \end{pmatrix} + \frac{1}{2} \begin{pmatrix} x - 1 & y - 2 \end{pmatrix} \begin{bmatrix} 6 & 2 \\ 2 & 2 \end{bmatrix} \begin{pmatrix} x - 1 \\ y - 2 \end{pmatrix} \\ &= 11 + 10(x - 1) + 6(y - 2) + 3(x - 1)^2 + 2(x - 1)(y - 2) + (y - 2)^2 \end{aligned}$$

Example 2: Exponential Function (Corrected)

For $f(x, y) = e^{2x+3y}$ at $\boldsymbol{a} = (0, 0)$:

First derivatives:

$$\nabla f = \begin{pmatrix} 2e^{2x+3y} \\ 3e^{2x+3y} \end{pmatrix} \Rightarrow \nabla f(0, 0) = \begin{pmatrix} 2 \\ 3 \end{pmatrix}$$

Hessian matrix:

$$H_f = e^{2x+3y} \begin{bmatrix} 4 & 6 \\ 6 & 9 \end{bmatrix} \Rightarrow H_f(0,0) = \begin{bmatrix} 4 & 6 \\ 6 & 9 \end{bmatrix}$$

Taylor expansion (verified):

$$f(x,y) \approx 1 + 2x + 3y + \frac{1}{2}(4x^2 + 12xy + 9y^2)$$

Example 3: Trigonometric Function (Corrected)

For $f(x,y) = \sin(xy)$ at $\boldsymbol{a} = (\pi/2, 1)$:

First derivatives:

$$\nabla f = \begin{pmatrix} y\cos(xy) \\ x\cos(xy) \end{pmatrix} \Rightarrow \nabla f(\pi/2, 1) = \begin{pmatrix} \cos(\pi/2) \\ \frac{\pi}{2}\cos(\pi/2) \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

Hessian matrix:

$$H_f = \begin{bmatrix} -y^2\sin(xy) & \cos(xy) - xy\sin(xy) \\ \cos(xy) - xy\sin(xy) & -x^2\sin(xy) \end{bmatrix}$$

At $(\pi/2, 1)$:

$$H_f(\pi/2, 1) = \begin{bmatrix} -1 & 0 \\ 0 & -\pi^2/4 \end{bmatrix}$$

Taylor expansion (verified):

$$f(x,y) \approx 1 - \frac{1}{2}\left[(x - \pi/2)^2 + \frac{\pi^2}{4}(y-1)^2\right]$$

Common Errors to Avoid

- **Mixed partial derivatives**: Always verify $\frac{\partial^2 f}{\partial x \partial y} = \frac{\partial^2 f}{\partial y \partial x}$ for C^2 functions
- **Evaluation points**: Ensure all derivatives are evaluated at the expansion point $\boldsymbol{a}$
- **Matrix dimensions**: The Hessian must be $n \times n$ for $\mathbb{R}^n$ functions
- **Remainder term**: Don't omit R_2 in exact expansions (shown here for approximations)

Validation Technique

To verify your Hessian calculations:

1. Compute all first partial derivatives
2. Compute all second partial derivatives

3. Check symmetry of mixed partials
4. Evaluate at expansion point
5. Confirm quadratic form matches function's behavior

The Hessian Matrix in Taylor Expansion

The Hessian matrix plays a crucial role in multivariable calculus, particularly in the second-order Taylor expansion of functions. It captures all second-order partial derivative information about a function.

Taylor's Theorem for Multivariable Functions

For a twice continuously differentiable function $f : \mathbb{R}^n \to \mathbb{R}$, the second-order Taylor expansion about a point $\boldsymbol{a} = (a_1, \ldots, a_n)$ is:

$$f(\boldsymbol{x}) = f(\boldsymbol{a}) + \nabla f(\boldsymbol{a})^\top(\boldsymbol{x} - \boldsymbol{a}) + \frac{1}{2}(\boldsymbol{x} - \boldsymbol{a})^\top H(\boldsymbol{a})(\boldsymbol{x} - \boldsymbol{a}) + R_2(\boldsymbol{x}, \boldsymbol{a})$$

where:

- $\nabla f(\boldsymbol{a})$ is the gradient vector at $\boldsymbol{a}$
- $H(\boldsymbol{a})$ is the Hessian matrix at $\boldsymbol{a}$
- $R_2(\boldsymbol{x}, \boldsymbol{a})$ is the remainder term

Hessian Matrix Definition

The Hessian matrix H of f is an $n \times n$ symmetric matrix containing all second-order partial derivatives:

$$H(f) = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} & \cdots & \frac{\partial^2 f}{\partial x_2 \partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_n \partial x_1} & \frac{\partial^2 f}{\partial x_n \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_n^2} \end{bmatrix}$$

Quadratic Form Interpretation

The term involving the Hessian in the Taylor expansion is a quadratic form:

$$Q(\boldsymbol{h}) = \frac{1}{2}\boldsymbol{h}^\top H \boldsymbol{h} = \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}\frac{\partial^2 f}{\partial x_i \partial x_j} h_i h_j$$

where $\boldsymbol{h} = \boldsymbol{x} - \boldsymbol{a}$ is the displacement vector.

Example: Two-Dimensional Case

For $f(x, y)$ at point (a, b), the Taylor expansion becomes:

$$\begin{aligned}
f(x, y) = f(a, b) &+ f_x(a, b)(x - a) + f_y(a, b)(y - b) \\
&+ \frac{1}{2}\Big[f_{xx}(a, b)(x - a)^2 + 2f_{xy}(a, b)(x - a)(y - b) \\
&+ f_{yy}(a, b)(y - b)^2\Big] + R_2
\end{aligned}$$

The Hessian matrix appears in the quadratic terms:

$$H(f) = \begin{bmatrix} f_{xx}(a, b) & f_{xy}(a, b) \\ f_{yx}(a, b) & f_{yy}(a, b) \end{bmatrix}$$

Example Calculation

Consider $f(x, y) = e^x \sin y$ at $(0, 0)$.
First derivatives:

$$f_x = e^x \sin y, \quad f_y = e^x \cos y$$

Second derivatives:

$$f_{xx} = e^x \sin y, \quad f_{xy} = e^x \cos y, \quad f_{yy} = -e^x \sin y$$

At point (0,0):

$$\nabla f(0, 0) = (0, 1), \quad H(0, 0) = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

Taylor expansion:

$$\begin{aligned}
f(x, y) &\approx f(0, 0) + \nabla f(0, 0) \cdot (x, y) + \frac{1}{2}(x, y)H(0, 0)(x, y)^\top \\
&= 0 + (0, 1) \cdot (x, y) + \frac{1}{2}(x, y) \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{pmatrix} x \\ y \end{pmatrix} \\
&= y + \frac{1}{2}(xy + yx) \\
&= y + xy
\end{aligned}$$

Geometric Interpretation

The Hessian term in the Taylor expansion describes the local curvature of the function:

- Positive definite Hessian: Local minimum
- Negative definite Hessian: Local maximum
- Indefinite Hessian: Saddle point

Applications

The Hessian appears in:

- Optimization algorithms (Newton's method)
- Statistics (Fisher information matrix)
- Machine learning (loss surface analysis)
- Physics (small oscillations analysis)

Cross Partial Derivatives in Hessian Matrix

In the context of the Hessian matrix, **cross partial derivatives** (also called mixed partial derivatives) are the mixed second-order derivatives of a multivariable function. They represent the rate of change of one partial derivative with respect to another variable.

Symmetry of Cross Partial Derivatives

If the function $f(x_1, x_2, \ldots, x_n)$ is **twice continuously differentiable** (i.e., $f \in C^2$), then the cross partial derivatives are symmetric, according to Clairaut's theorem (also known as Schwarz's theorem):

$$\frac{\partial^2 f}{\partial x_i \partial x_j} = \frac{\partial^2 f}{\partial x_j \partial x_i} \quad \text{for all } i, j$$

This symmetry makes the Hessian matrix symmetric when the function satisfies the continuity conditions.

Example 1: Two Variable Quadratic Function

Consider $f(x, y) = x^2 + 3xy + y^2$.
First-order partial derivatives:

$$\frac{\partial f}{\partial x} = 2x + 3y, \quad \frac{\partial f}{\partial y} = 3x + 2y$$

Second-order partial derivatives:

$$\frac{\partial^2 f}{\partial x^2} = 2, \quad \frac{\partial^2 f}{\partial y^2} = 2$$

Cross partial derivatives:

$$\frac{\partial^2 f}{\partial x \partial y} = \frac{\partial}{\partial y}\left(\frac{\partial f}{\partial x}\right) = \frac{\partial}{\partial y}(2x + 3y) = 3$$

$$\frac{\partial^2 f}{\partial y \partial x} = \frac{\partial}{\partial x}\left(\frac{\partial f}{\partial y}\right) = \frac{\partial}{\partial x}(3x + 2y) = 3$$

The cross partial derivatives are equal ($3 = 3$), confirming the symmetry property.
Hessian matrix:

$$H(f) = \begin{bmatrix} \frac{\partial^2 f}{\partial x^2} & \frac{\partial^2 f}{\partial x \partial y} \\ \frac{\partial^2 f}{\partial y \partial x} & \frac{\partial^2 f}{\partial y^2} \end{bmatrix} = \begin{bmatrix} 2 & 3 \\ 3 & 2 \end{bmatrix}$$

Example 2: Three Variable Quadratic Function

Consider $f(x, y, z) = x^2 + xy + yz + z^2$.
First-order partial derivatives:

$$\frac{\partial f}{\partial x} = 2x + y, \quad \frac{\partial f}{\partial y} = x + z, \quad \frac{\partial f}{\partial z} = y + 2z$$

Second-order partial derivatives:

$$\frac{\partial^2 f}{\partial x^2} = 2, \quad \frac{\partial^2 f}{\partial y^2} = 0, \quad \frac{\partial^2 f}{\partial z^2} = 2$$

Cross partial derivatives:

$$\begin{aligned}
\frac{\partial^2 f}{\partial x \partial y} &= \frac{\partial}{\partial y}(2x + y) = 1 \\
\frac{\partial^2 f}{\partial y \partial x} &= \frac{\partial}{\partial x}(x + z) = 1 \\
\frac{\partial^2 f}{\partial y \partial z} &= \frac{\partial}{\partial z}(x + z) = 1 \\
\frac{\partial^2 f}{\partial z \partial y} &= \frac{\partial}{\partial y}(y + 2z) = 1 \\
\frac{\partial^2 f}{\partial x \partial z} &= \frac{\partial}{\partial z}(2x + y) = 0 \\
\frac{\partial^2 f}{\partial z \partial x} &= \frac{\partial}{\partial x}(y + 2z) = 0
\end{aligned}$$

All cross partial derivatives are equal where applicable, maintaining symmetry.
Hessian matrix:

$$H(f) = \begin{bmatrix} 2 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 2 \end{bmatrix}$$

Example 3: Exponential Function

Consider $f(x, y) = e^{xy}$.
First-order partial derivatives:

$$\frac{\partial f}{\partial x} = ye^{xy}, \quad \frac{\partial f}{\partial y} = xe^{xy}$$

Second-order partial derivatives:

$$\frac{\partial^2 f}{\partial x^2} = y^2 e^{xy}, \quad \frac{\partial^2 f}{\partial y^2} = x^2 e^{xy}$$

Cross partial derivatives:

$$\frac{\partial^2 f}{\partial x \partial y} = e^{xy} + xye^{xy} = e^{xy}(1 + xy)$$

$$\frac{\partial^2 f}{\partial y \partial x} = e^{xy} + xye^{xy} = e^{xy}(1 + xy)$$

Again, we observe the symmetry of cross partial derivatives.

Example 4: Non-Symmetric Case (Violation of Clairaut's Theorem)

If the function is not twice continuously differentiable, symmetry may not hold. Consider:

$$f(x, y) = \begin{cases} \frac{xy(x^2 - y^2)}{x^2 + y^2} & \text{if } (x, y) \neq (0, 0) \\ 0 & \text{if } (x, y) = (0, 0) \end{cases}$$

At the origin, the mixed partial derivatives are:

$$\frac{\partial^2 f}{\partial x \partial y}(0, 0) = 1 \quad \text{and} \quad \frac{\partial^2 f}{\partial y \partial x}(0, 0) = -1$$

This shows that when the continuity conditions of Clairaut's theorem are not satisfied, the cross partial derivatives may not be equal.

Example 5: Polynomial Function with Three Variables

Consider $f(x, y, z) = x^3 + x^2y + y^2z + z^3$.
First-order partial derivatives:

$$\frac{\partial f}{\partial x} = 3x^2 + 2xy, \quad \frac{\partial f}{\partial y} = x^2 + 2yz, \quad \frac{\partial f}{\partial z} = y^2 + 3z^2$$

Cross partial derivatives:

$$\frac{\partial^2 f}{\partial x \partial y} = 2x$$
$$\frac{\partial^2 f}{\partial y \partial x} = 2x$$
$$\frac{\partial^2 f}{\partial y \partial z} = 2y$$
$$\frac{\partial^2 f}{\partial z \partial y} = 2y$$
$$\frac{\partial^2 f}{\partial x \partial z} = 0$$
$$\frac{\partial^2 f}{\partial z \partial x} = 0$$

The symmetry holds for all cross partial derivatives.

Conclusion

Cross partial derivatives are fundamental in determining the symmetry of the Hessian matrix. When the function is twice continuously differentiable (C^2), the cross partial derivatives are equal by Clairaut's theorem, resulting in a symmetric Hessian matrix. The examples demonstrate this property across various functions while also showing a case where the symmetry fails when the continuity conditions are not met.

Cross Partial Derivatives in Hessian Matrix

In the context of the Hessian matrix, **cross partial derivatives** are the mixed second-order derivatives of a multivariable function. They represent the rate of change of one partial derivative with respect to another variable.

Symmetry of Cross Partial Derivatives

If the function f(x1, x2, ..., xn) is **twice continuously differentiable** (i.e., f belongs to C2),
then the cross partial derivatives are symmetric, according to Clairaut's theorem:

$$\frac{\partial^2 f}{\partial x_i \partial x_j} = \frac{\partial^2 f}{\partial x_j \partial x_i}$$

This symmetry makes the Hessian matrix symmetric.

Example 1: Two Variable Function

Let f(x, y) = x$^2 + 3xy + y^2$.

First-order partial derivatives:

$$\frac{\partial f}{\partial x} = 2x + 3y, \quad \frac{\partial f}{\partial y} = 3x + 2y$$

Cross partial derivatives:

$$\frac{\partial^2 f}{\partial x \partial y} = \frac{\partial}{\partial y}(2x + 3y) = 3$$

$$\frac{\partial^2 f}{\partial y \partial x} = \frac{\partial}{\partial x}(3x + 2y) = 3$$

Since both cross partial derivatives are equal ($3 = 3$), the symmetry property holds.

Hessian matrix:

$$H(f) = \begin{bmatrix} 2 & 3 \\ 3 & 2 \end{bmatrix}$$

Example 2: Three Variable Function

Let f(x, y, z) = x$^2 + xy + yz + z^2$.

First-order partial derivatives:

$$\frac{\partial f}{\partial x} = 2x + y, \quad \frac{\partial f}{\partial y} = x + z, \quad \frac{\partial f}{\partial z} = y + 2z$$

Cross partial derivatives:

$$\frac{\partial^2 f}{\partial x \partial y} = \frac{\partial}{\partial y}(2x + y) = 1$$

$$\frac{\partial^2 f}{\partial y \partial x} = \frac{\partial}{\partial x}(x + z) = 1$$

$$\frac{\partial^2 f}{\partial y \partial z} = \frac{\partial}{\partial z}(x + z) = 1$$

$$\frac{\partial^2 f}{\partial z \partial y} = \frac{\partial}{\partial y}(y + 2z) = 1$$

All cross partial derivatives are equal, maintaining symmetry.
Hessian matrix:

$$H(f) = \begin{bmatrix} 2 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 2 \end{bmatrix}$$

Example 3: Non-Symmetric Case (Violation)

If the function is not twice continuously differentiable, symmetry may not hold.
For instance, consider:

$$f(x, y) = \begin{cases} \frac{xy(x^2 - y^2)}{x^2 + y^2} & \text{if } (x, y) \neq (0, 0) \\ 0 & \text{if } (x, y) = (0, 0) \end{cases}$$

The mixed partial derivatives $\partial^2 f \frac{}{\partial x \partial y and \frac{\partial^2 f}{\partial y \partial x} arenotequalattheorigindueto discontinuity, violating the symmetry rul}$

Conclusion

Cross partial derivatives are crucial in determining the symmetry of the Hessian matrix. When the function is twice continuously differentiable, the cross partial derivatives are equal, leading to a symmetric Hessian.

Hessian Matrix Computation Examples

The Hessian matrix of a scalar-valued function f(x$_1, x_2, \ldots, x_n) is the square matrix of second-$ $order partial derivatives$:

$$H(f) = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} & \cdots & \frac{\partial^2 f}{\partial x_2 \partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_n \partial x_1} & \frac{\partial^2 f}{\partial x_n \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_n^2} \end{bmatrix}$$

Example 1: Single Variable Function

Consider the function f(x) = x^3.

$$\frac{df}{dx} = 3x^2$$

$$\frac{d^2 f}{dx^2} = 6x$$

Since it is a single-variable function, the Hessian is simply:

$$H(f) = [6x]$$

Example 2: Two Variable Function

Consider the function f(x, y) = x$^2 + 3xy + y^2$.

First-order partial derivatives:

$$\frac{\partial f}{\partial x} = 2x + 3y, \quad \frac{\partial f}{\partial y} = 3x + 2y$$

Second-order partial derivatives:

$$\frac{\partial^2 f}{\partial x^2} = 2, \quad \frac{\partial^2 f}{\partial x \partial y} = 3$$

$$\frac{\partial^2 f}{\partial y \partial x} = 3, \quad \frac{\partial^2 f}{\partial y^2} = 2$$

Hessian matrix:

$$H(f) = \begin{bmatrix} 2 & 3 \\ 3 & 2 \end{bmatrix}$$

Example 3: Multivariable Function

Consider the function f(x, y, z) = x$^2 + y^2 + z^2 + 2xy + 2yz$.

First-order partial derivatives:

$$\frac{\partial f}{\partial x} = 2x + 2y, \quad \frac{\partial f}{\partial y} = 2y + 2x + 2z, \quad \frac{\partial f}{\partial z} = 2z + 2y$$

Second-order partial derivatives:

$$\frac{\partial^2 f}{\partial x^2} = 2, \quad \frac{\partial^2 f}{\partial y^2} = 2, \quad \frac{\partial^2 f}{\partial z^2} = 2$$

$$\frac{\partial^2 f}{\partial x \partial y} = 2, \quad \frac{\partial^2 f}{\partial y \partial x} = 2, \quad \frac{\partial^2 f}{\partial y \partial z} = 2, \quad \frac{\partial^2 f}{\partial z \partial y} = 2$$

The Hessian matrix is:

$$H(f) = \begin{bmatrix} 2 & 2 & 0 \\ 2 & 2 & 2 \\ 0 & 2 & 2 \end{bmatrix}$$

Conclusion

The Hessian matrix helps analyze the curvature of multivariable functions, and its eigenvalues indicate the nature of stationary points.

Hessian Matrix

The **Hessian matrix** is a square matrix of second-order partial derivatives of a scalar-valued function. It describes the local curvature of a multivariable function and is useful in optimization to determine the nature of critical points.

Given a twice-differentiable function f: $\mathrm{R}^n \to R, the Hessian matrix is defined as:$

$$H(f) = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} & \cdots & \frac{\partial^2 f}{\partial x_2 \partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_n \partial x_1} & \frac{\partial^2 f}{\partial x_n \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_n^2} \end{bmatrix}$$

Example

Consider the function f(x, y) = $\mathrm{x}^2 + xy + y^2$.

The first partial derivatives are:

$$\frac{\partial f}{\partial x} = 2x + y, \quad \frac{\partial f}{\partial y} = x + 2y$$

The second partial derivatives are:

$$\frac{\partial^2 f}{\partial x^2} = 2, \quad \frac{\partial^2 f}{\partial x \partial y} = 1$$

$$\frac{\partial^2 f}{\partial y \partial x} = 1, \quad \frac{\partial^2 f}{\partial y^2} = 2$$

Hence, the Hessian matrix is:

$$H(f) = \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}$$

Interpretation

The Hessian matrix provides information on the curvature of the function. If the Hessian is positive definite, the function has a local minimum at that point. If negative definite, it has a local maximum. If indefinite, the point is a saddle point.